

Second Edition

HANDBOOK OF

Physical-Chemical Properties and Environmental Fate for Organic Chemicals

Volume I

Introduction and Hydrocarbons

Volume II

Halogenated Hydrocarbons

Volume III

Oxygen Containing Compounds

Volume IV

Nitrogen and Sulfur Containing Compounds
and Pesticides

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Donald Mackay

Wan Ying Shiu

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Preface

This handbook is a compilation of environmentally relevant physical-chemical data for similarly structured groups of chemical substances. These data control the fate of chemicals as they are transported and transformed in the multimedia environment of air, water, soils, sediments, and their resident biota. These fate processes determine the exposure experienced by humans and other organisms and ultimately the risk of adverse effects. The task of assessing chemical fate locally, regionally, and globally is complicated by the large (and increasing) number of chemicals of potential concern; by uncertainties in their physical-chemical properties; and by lack of knowledge of prevailing environmental conditions such as temperature, pH, and deposition rates of solid matter from the atmosphere to water, or from water to bottom sediments. Further, reported values of properties such as solubility are often in conflict. Some are measured accurately, some approximately, and some are estimated by various correlation schemes from molecular structures. In some cases, units or chemical identity are wrongly reported. The user of such data thus has the difficult task of selecting the “best” or “right” values. There is justifiable concern that the resulting deductions of environmental fate may be in substantial error. For example, the potential for evaporation may be greatly underestimated if an erroneously low vapor pressure is selected.

To assist the environmental scientist and engineer in such assessments, this handbook contains compilations of physical-chemical property data for over 1000 chemicals. It has long been recognized that within homologous series, properties vary systematically with molecular size, thus providing guidance about the properties of one substance from those of its homologs. Where practical, plots of these systematic property variations can be used to check the reported data and provide an opportunity for interpolation and even modest extrapolation to estimate unmeasured properties of other substances. Most handbooks treat chemicals only on an individual basis and do not contain this feature of chemical-to-chemical comparison, which can be valuable for identifying errors and estimating properties. This most recent edition includes about 1250 compounds and contains about 30 percent additional physical-chemical property data. There is a more complete coverage of PCBs, PCDDs, PCDFs, and other halogenated hydrocarbons, especially brominated and fluorinated substances that are of more recent environmental concern. Values of the physical-chemical properties are generally reported in the literature at a standard temperature of 20 or 25°C. However, environmental temperatures vary considerably, and thus reliable data are required on the temperature dependence of these properties for fate calculations. A valuable enhancement to this edition is the inclusion of extensive measured temperature-dependent data for the first time. The data focus on water solubility, vapor pressure, and Henry’s law constant but include octanol/water and octanol/air partition coefficients where available. They are provided in the form of data tables and correlation equations as well as graphs.

We also demonstrate in [Chapter 1](#) how the data may be taken a stage further and used to estimate likely environmental partitioning tendencies, i.e., how the chemical is likely to become distributed between the various media that comprise our biosphere. The results are presented numerically and pictorially to provide a visual impression of likely environmental behavior. This will be of interest to those assessing environmental fate by confirming the general fate characteristics or behavior profile. It is, of course, only possible here to assess fate in a “typical” or “generic” or “evaluative” environment. No claim is made that a chemical will behave in this manner in all situations, but this assessment should reveal the broad characteristics of behavior. These evaluative fate assessments are generated using simple fugacity models that flow naturally from the compilations of data on physical-chemical properties of relevant chemicals. Illustrations of estimated environmental fate are given in Chapter 1 using Levels I, II, and III mass balance models. These and other models are available for downloading gratis from the website of the Canadian Environmental Modelling Centre at Trent University (www.trent.ca/cemc).

It is hoped that this new edition of the handbook will be of value to environmental scientists and engineers and to students and teachers of environmental science. Its aim is to contribute to better assessments of chemical fate in our multimedia environment by serving as a reference source for environmentally relevant physical-chemical property data of classes of chemicals and by illustrating the likely behavior of these chemicals as they migrate throughout our biosphere.

Acknowledgments

We would never have completed the volumes for the first and second editions of the handbook and the CD-ROMs without the enormous amount of help and support that we received from our colleagues, publishers, editors, friends, and family. We are long overdue in expressing our appreciation.

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Much credit goes to the team of professionals at CRC Press/Taylor & Francis Group who worked on this second edition. Especially important were Dr. Fiona Macdonald, Publisher, Chemistry; Dr. Janice Shackleton, Input Supervisor; Patricia Roberson, Project Coordinator; Elise Oranges and Jay Margolis, Project Editors; and Marcela Peres, Production Assistant.

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Biographies

Donald Mackay, born and educated in Scotland, received his degrees in Chemical Engineering from the University of Glasgow. After working in the petrochemical industry he joined the University of Toronto, where he taught for 28 years in the Department of Chemical Engineering and Applied Chemistry and in the Institute for Environmental Studies. In 1995 he moved to Trent University to found the Canadian Environmental Modelling Centre. Professor Mackay's primary research is the study of organic environmental contaminants, their properties, sources, fates, effects, and control, and particularly understanding and modeling their behavior with the aid of the fugacity concept. His work has focused especially on the Great Lakes Basin; on cold northern climates; and on modeling bioaccumulation and chemical fate at local, regional, continental and global scales.

His awards include the SETAC Founders Award, the Honda Prize for Eco-Technology, the Order of Ontario, and the Order of Canada. He has served on the editorial boards of several journals and is a member of SETAC, the American Chemical Society, and the International Association of Great Lakes Research.

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10.1 LIST OF CHEMICALS AND DATA COMPILATIONS

10.1.1 ALIPHATIC ETHERS

10.1.1.1 Dimethyl ether (Methyl ether)



Common Name: Dimethyl ether

Synonym: methyl ether, oxapropane, oxybismethane

Chemical Name: dimethyl ether, methyl ether,

CAS Registry No: 115-10-6

Molecular Formula: C_2H_6O , CH_3OCH_3

Molecular Weight: 46.068

Melting Point ($^{\circ}C$):

–138.5 (Stull 1947; Stephenson & Malanowski 1987)

–141.5 (Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

–24.75 (Ambrose et al. 1976)

–23.60 (Stephenson & Malanowski 1987)

–24.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.6689 (Riddick et al. 1986)

0.6612 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.87 ($20^{\circ}C$, calculated-density)

60.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

4.941 (Riddick et al. 1986; Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

71000 (Seidell 1941; Lange 1971)

35.3% ($24^{\circ}C$, selected, Riddick et al. 1986)

65200 (literature data compilation, Yaws et al. 1990)

47480 (calculated- V_M , Wang et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

100847* ($-24.91^{\circ}C$, static method-manometer, measured range -78.22 to $-24.91^{\circ}C$, Kennedy et al. 1941)

678090* (calculated-Antoine eq. regression, temp range -115.7 to $-23.7^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 5409.8/(T/K)] + 7.585479$; temp range -115.7 to $125.2^{\circ}C$ (Antoine eq., Weast 1972–73)

593300 (Ambrose et al. 1976, Riddick et al. 1986)

$\log(P/kPa) = 6.0823 - 882.52/\{(T/K) + 31.90\}$ (Antoine eq., Ambrose et al. 1976)

$\log(P/mmHg) = 6.97603 - 889.3645/(241.96 + t/^{\circ}C)$; temp range -71 to $-25^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P/kPa) = 5.44136 - 1025.56/(256.05 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

575530, 593340 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.44136 - 1025.56/(-17.1 + T/K)$; temp range 183–265 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.30358 - 982.46/(-20.894 + T/K)$, temp range not specified (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.36332 - 995.747/(-19.864 + T/K)$; temp range 180–249 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.09354 - 880.813/(-33.007 + T/\text{K})$; temp range 241–303 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.28318 - 987.484/(-16.813 + T/\text{K})$; temp range 293–360 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.48877 - 1971.127/(122.787 + T/\text{K})$; temp range 349–400 K (Antoine eq.-VI, Stephenson & Malanowski 1987)

374000* (10°C, vapor-liquid equilibrium, measured range 203.15–395 K, Noles & Zollweg 1992)

$\log (P/\text{mmHg}) = 20.2699 - 1.5914 \times 10^3/(T/\text{K}) - 4.653 \cdot \log (T/\text{K}) - 1.3178 \times 10^{-10} \cdot (T/\text{K}) + 2.5623 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 132–400 K (vapor pressure eq., Yaws et al. 1994)

510000* (20.5°C, vapor-liquid equilibrium, measured range 0.51–120.12°C, Jónasson et al. 1995)

589100 (25.02°C, vapor-liquid equilibrium, measured range 283.12–313.22 K, Bobbo et al. 2000)

596210* (25.022°C, static-pressure sensor, measured range 233–399 K, data fitted to Wagner type eq., Wu et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

101.0 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

49.5, 105.7 (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.10 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1987)

0.10 (recommended, Sangster 1989)

0.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

1.37 (calculated- S_{oct} and vapor pressure P , Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{O_3(P)} = 5.7 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $O_3(P)$ at room temp. (Gaffney & Levine 1979)

$k_{OH}^* = 3.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298.9 K, measured range 298–505 K (flash photolysis-resonance fluorescence, Perry et al. 1977)

$k_{OH}(\text{calc}) = 2.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{NO_3} \leq 3.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (flash photolysis-visible absorption, Wallington et al. 1986; quoted, Sabljic & Güsten 1990; Atkinson 1991)

$k_{OH}^* = 2.95 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–442 K (Tully & Droege 1987)

$k_{NO_3} = 2.92 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Sabljic & Güsten 1990)

$k_{OH}(\text{exptl}) = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (24.9 \pm 2.2) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)

$k_{OH} = 2.49 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{OH}^* = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (2.35 \pm 0.24) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (3.19 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}^* = 2.95 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–650 K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)

$k_{\text{OH}}^* = 2.86 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 263–351 K (relative rate method, DeMore & Bayes 1999)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976); calculated lifetimes of 4.1 d and 180 d for reactions with OH radical, NO_3 radical, respectively (Atkinson .2000)

TABLE 10.1.1.1.1

Reported vapor pressures of dimethyl ether at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
$\log P = A - B/(T/K) + C \cdot \log (T/K) - D \cdot (T/K)$	(5)						
1.							
Kennedy et al. 1941	Stull 1947	Jónasson et al. 1995	Wu et al. 2004				
static method-manometer	summary of literature data	static-pressure gauge	quartz pressure sensors				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
−78.22	4684	−115.7	133.3	0.51	270000	233.128	54610
−70.66	8121	−101.1	666.6	3.07	300000	238.126	68490
−65.25	11706	−93.3	1333	4.97	330000	243.157	85570
−60.03	16315	−85.2	2666	15.01	430000	248.152	105590
−55.14	21910	−76.2	5333	20.50	510000	253.152	129.42
−49.90	29585	−70.4	7999	27.11	630000	258.160	157530
−45.10	38334	−62.7	13332	33.39	750000	263.160	190440
−40.02	49810	−50.0	26664	44.39	990000	268.161	228480
−35.10	63401	−37.8	53329	50.25	1160000	273.153	272170
−27.67	89362	−23.7	101325	63.94	1590000	278.145	321870
−24.91	100847			76.67	2080000	283.160	378660
		mp/°C	−138.5	89.25	2680000	288.174	444570
mp/°C	−141.5			103.77	3500000	293.161	515530
bp/°C	−24.82			120.12	4720000	298.172	596210
		Noles & Zollweg 1992				303.160	687370
		vapor-liquid equilibrium				305.160	726260
eq. 5	P/mmHg	t/°C	P/Pa			308.158	787070
A	23.686185	10	37400			313.156	897590
B	1691.8056	50	114900			316.154	968550
C	−6.04560	90	273800			318.158	1018910
D	0.00195754	99.95	328400			323.149	1152350
temp range 195–284.34 K		109.85	357000			328.149	1298230
		121.85	488200			333.157	1457500
						more to	
						400.378	5355800
						data fitted to Wagner eq.	

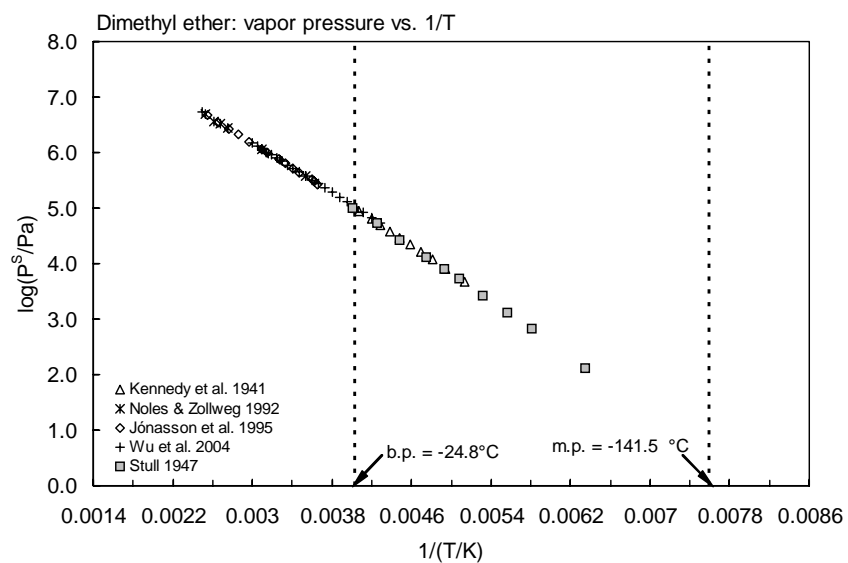
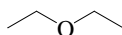


FIGURE 10.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl ether.

10.1.1.2 Diethyl ether (Ethyl ether)



Common Name: Diethyl ether

Synonym: ether, ethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1'-oxybisethane, sulfuric ether

Chemical Name: ether, diethyl ether, ethoxyethane, ethyl oxide, 3-oxapentane, 1,1'-oxybisethane

CAS Registry No: 60-29-7

Molecular Formula: $C_4H_{10}O$, $CH_3CH_2OCH_2CH_3$

Molecular Weight: 74.121

Melting Point ($^{\circ}C$):

-116.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

34.5 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7136. 0.7078 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.9 ($20^{\circ}C$, calculated-density)

106.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.439 (quoted, Riddick et al. 1986)

7.19 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

60270* (thermostatic volumetric method, measured range -3.83 to $30^{\circ}C$, Hill 1923)

60400* (volumetric method, measured range 10 – $30^{\circ}C$, Kablukov & Malischeva 1925)

60300* (volumetric method, measured range 10 – $25^{\circ}C$, Bennett & Phillip 1928)

69000 (Seidell 1941; Lange 1971)

60400 (selected, Riddick et al. 1986)

60900 (literature data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

58335* ($19.871^{\circ}C$, manometer, measured range -60.799 – $19.871^{\circ}C$, Taylor & Smith)

74690* (calculated-Antoine eq. regression, temp range -74 to $35.6^{\circ}C$, Stull 1947)

323835* ($71.11^{\circ}C$, static method-Bourdon, measured range 71.11 – $187.78^{\circ}C$, Kobe et al. 1956)

$\log (P/mmHg) = [-0.2185 \times 6946.2/(T/K)] + 7.56659$; temp range -74.3 to $183.3^{\circ}C$ (Antoine eq., Weast 1972–73)

58920 ($20^{\circ}C$, Verschueren 1983)

63340* ($21.82^{\circ}C$, ebulliometry, measured range 250 – $467 K$, Ambrose et al. 1972; quoted, Boublik et al. 1984)

$\log (P/kPa) = 6.05115 - 1062.409/[(T/K) - 44.967]$; temp range 250 – $329 K$ (ebulliometry, Antoine eq., Ambrose et al. 1972)

71620 (Ambrose et al. 1976)

71240, 71610 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.04972 - 1066.052/(220.003 + t/^{\circ}C)$; temp range -70.0 to $19.87^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.0492 - 1061.391/(228.06 + t/^{\circ}C)$; temp range -23.1 to $55.434^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1972, Boublik et al. 1984)

$\log (P/mmHg) = 6.92032 - 1064.07/(228.8 + t/^{\circ}C)$; temp range -61 to $20^{\circ}C$ (Antoine eq., Dean 1985, 1992)

71620 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.05115 - 1062.409/(228.183 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
71620, 71604 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.02962 - 1051.432/(-44.967 + T/\text{K})$; temp range 286–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.05115 - 1062.409/(-44.967 + T/\text{K})$; temp range 250–329 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.30714 - 1236.75/(-20.11 + T/\text{K})$; temp range 307–457 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.05933 - 1067.576/(-44.217 + T/\text{K})$; temp range 305–360 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.37811 - 1276.822/(-14.869 + T/\text{K})$; temp range 417–467 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 41.7519 - 2.741 \times 10^3/(T/\text{K}) - 12.27 \cdot \log (T/\text{K}) - 3.1948 \times 10^{-10} \cdot (T/\text{K}) + 5.9802 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 157–467 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence):

130 (calculated- $1/K_{\text{AW}}$, $C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

90.0 (calculated-group contribution method, Hine & Mookerjee 1975)

237 (calculated-bond contribution method, Hine & Mookerjee 1975)

87.9 (calculated-P/C using Riddick et al. 1986 data)

86.8 (23°C , batch air stripping-IR, Nielsen et al. 1994)

95.05 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{\text{AW}} = 5.953 - 2158/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.83 (20°C , shake flask-CR, Collander 1951)

1.03 (Hansch et al. 1968)

0.89 (shake flask-GC, both phases, Hansch et al. 1975)

0.77 (shake flask, Log P Database, Hansch & Leo 1987)

0.89 (recommended, Sangster 1989)

0.89 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C :

2.19 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}}(\text{calc}) = 1.43 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.34 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = 13.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K, measured range 295–442 K (Tully & Droege 1987)

$k_{\text{OH}}(\text{exptl}) = 1.34 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 1.06 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}}^* = (13.6 \pm 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988b)

$k_{\text{OH}} = 1.36 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{\text{OH}} = 1.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (relative rate method, Bennett & Keer 1989)

$k_{\text{OH}}^* = 1.33 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}} = (11.3 \pm 0.10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{\text{OH}} = (12.8 \pm 0.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from the air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetimes of 11 h and 17 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

TABLE 10.1.1.2.1

Reported aqueous solubilities of diethyl ether at various temperatures

Hill 1923		Kablukov & Malischeva 1925		Bennett & Phillip 1928	
volumetric method		volumetric method		volumetric method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
-3.83	127520	10	90100	10	91000
0	116680	15	78700	15	79500
10	90400	20	68800	20	68700
15	79130	25	60400	25	60300
20	68960	30	53400		
25	60270				
30	53400				

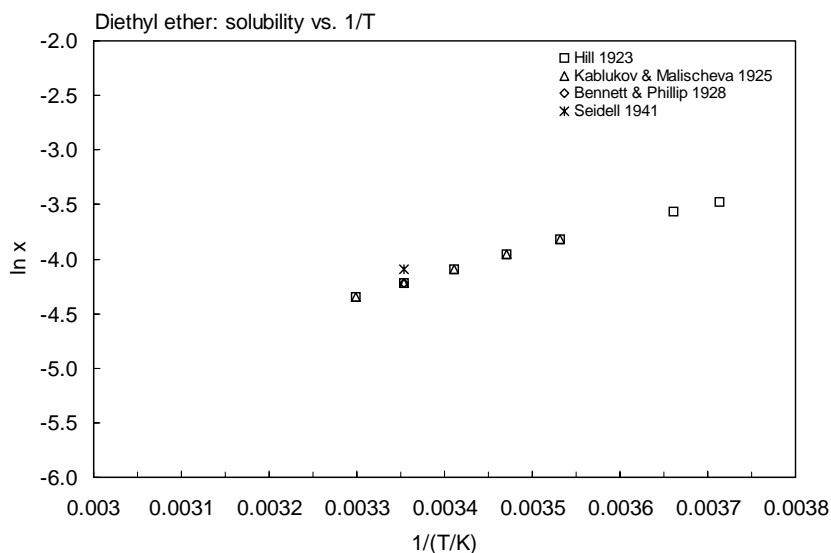


FIGURE 10.1.1.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for diethyl ether.

TABLE 10.1.1.2.2

Reported vapor pressures of diethyl ether at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Taylor & Smith 1922		Stull 1947		Kobe et al. 1956		Ambrose et al. 1972	
manometer		summary of literature data		static method-Bourdon gauge		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−60.799	527	−20.4	133.3	71.11	323835	−23.104	7430
−55.748	791	−3.0	666.6	76.67	372065	−19.889	8933
−50.873	1169	5.5	1333	82.22	427186	−16.744	10619
−45.998	1683	14.3	2666	87.78	496087	−13.492	12664
−41.125	2370	24.5	5333	93.33	564988	−10.135	15090
−36.231	3302	31.0	7999	98.89	647669	−6.929	17753
−31.329	4537	39.8	13332	104.44	730351	−2.762	21778
−26.421	6107	52.7	26664	110.00	826812	0.828	25813
−21.502	8174	68.0	53329	115.56	923273	4.912	31134
−16.578	10755	82.9	101325	121.11	1040405	8.914	37179
−11.637	13971	mp/°C	25.3	126.67	1157537	13.137	44534
−6.698	17966			132.22	1288449	17.785	53941
0.009	24815			137.78	1426251	21.821	63.343
4.975	31161			143.33	1584723	26.115	74719
9.937	38746			148.89	1743195	30.764	88.801
14.093	47749			154.44	1929288	34.321	100931
19.871	58335			160.00	2122151	35.064	103618
				165.56	2287513	39.222	119720
				171.11	2542447	42.978	135889
				176.67	2797381	47.470	157395
		182.22	3059204	51.765	180321		
		187.78	3341699	55.434	201878		
						eq. 3	P/kPa
						A	6.05115
						B	1062.409
						C	−44.967

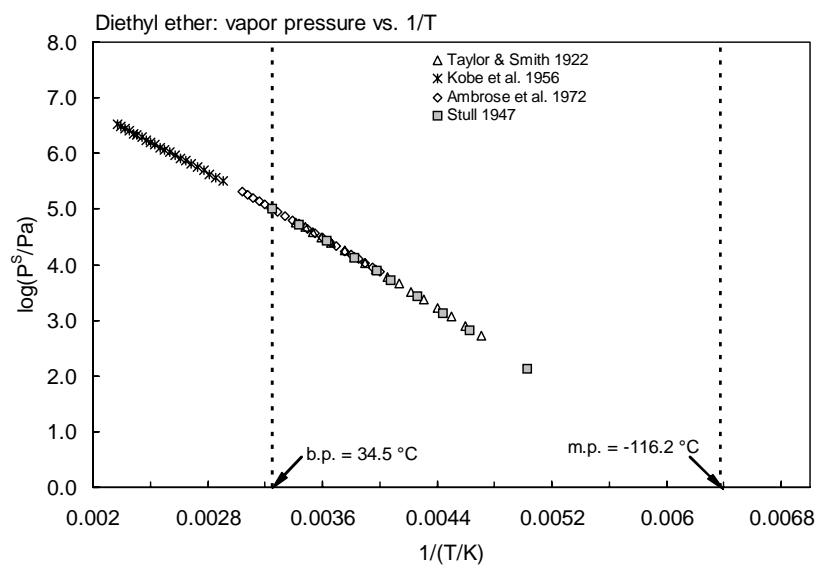


FIGURE 10.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl ether.

10.1.1.3 Methyl *t*-butyl ether (MTBE)



Common Name: Methyl *t*-butyl ether

Synonym: MTBE, 3-oxa-3,3-dimethylbutane, 2-methoxy-2-methyl-propane

Chemical Name: methyl *tert*-butyl ether

CAS Registry No: 1634-04-4

Molecular Formula: C₅H₁₂O, CH₃-O-C(CH₃)₃

Molecular Weight: 88.148

Melting Point (°C):

-108.6 (Lide 2003)

Boiling Point (°C):

55.0 (Lide 2003)

Density (g/cm³ at 20°C):

0.7578 (Bennett & Phillip 1928)

0.7404 (Windholz 1983; Budavari 1989)

Molar Volume (cm³/mol):

119.1 (20°C, calculated-density)

127.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

7.60 (exptl., Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

51600* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)

48000 (Windholz 1983; Budavari 1989)

52100 (literature data compilation, Yaws et al. 1990)

42000* (19.8°C, shake flask-GC/TC, measured range 0–48.6°C, Stephenson 1992)

62100, 35500 (5, 20°C, shake flask-GC, Fischer et al. 2004)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

31156* (23.243°C, comparative ebulliometry, measured range 288–351 K, Ambrose et al. 1976)

log (P/kPa) = 6.09379 – 1173.036/{(T/K) + 41.366}; temp range 288–351 K (Antoine equation, comparative ebulliometry, Ambrose et al. 1976)

32660 (Windholz 1983; Budavari 1989)

33545 (calculated-Antoine eq., Stephenson & Malanowski 1987)

log (P₁/kPa) = 6.09111 – 1171.54/(–41.542 + T/K); temp range 287–351 K (Antoine eq., Stephenson & Malanowski 1987)

37417* (27.806°C, static method, measured range 301–411 K, Krähenbühl & Gmehling 1994)

log (P/kPa) = 6.070343 – 1158.923/(T/K) – 43.20; temp range 301–411 K (Antoine eq., static method, Krähenbühl & Gmehling 1994)

log (P/mmHg) = 4.7409 – 1.9493 × 10³/(T/K) + 3.077 · log (T/K) – 1.4463 × 10⁻² · (T/K) + 1.0039 × 10⁻⁵ · (T/K)²; temp range 165–497 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equation. Additional data at other temperatures designated * are compiled at the end of this section):

59.46 (calculated as 1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)

142.6, 305 (calculated-group contribution, calculated-bond contribution method, Hine & Mookerjee 1975)

53.54*, 121 (25, 30°C, static headspace-GC, Robbins et al. 1993)

63.2 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

137.6* (solid-phase microextraction-GC, measured range 15–40°C, Bierwagen & Keller 2001)

$\ln K_{AW} = 6.6475 - 2901.4/(T/K)$; temp range 15–40°C (SPME-GC, Bierwagen & Keller 2001)

41.2 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 9.070 - 3178/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

72.4* (equilibrium concentration ratio-GC, measured range 3–25°C, Fischer et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.06 (Hansch et al. 1968; Kier & Hall 1976)

1.30 (calculated-fragment const., Hansch & Leo 1979)

0.94 (shake flask-GC, Funasaki et al. 1985)

0.94 (recommended, Sangster 1989)

0.94 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH}(\text{calc}) = 1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{exptl}) = 2.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (3.09 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 3.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 2.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 2.83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = (2.44 - 3.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295–298 K (Atkinson 1989)

$k_{OH}^* = 2.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 293 K, measured range 293–750 K (laser photolysis-laser induced fluorescence technique, Arif et al. 1997)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated lifetimes of 3.9 d and 72 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

TABLE 10.1.1.3.1

Reported aqueous solubilities of methyl *tert*-butyl ether (MTBE) at various temperatures

Bennett & Phillip 1928		Stephenson 1992		Fischer et al. 2004	
volumetric method		shake flask-GC/TC		shake flask-GC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	91200	0	83000	5	62100
10	73000	9.7	51000	20	35500
15	65500	19.8	42000		
20	58300	29.6	31000		
25	51600	39.3	25000		
		48.6	19000		

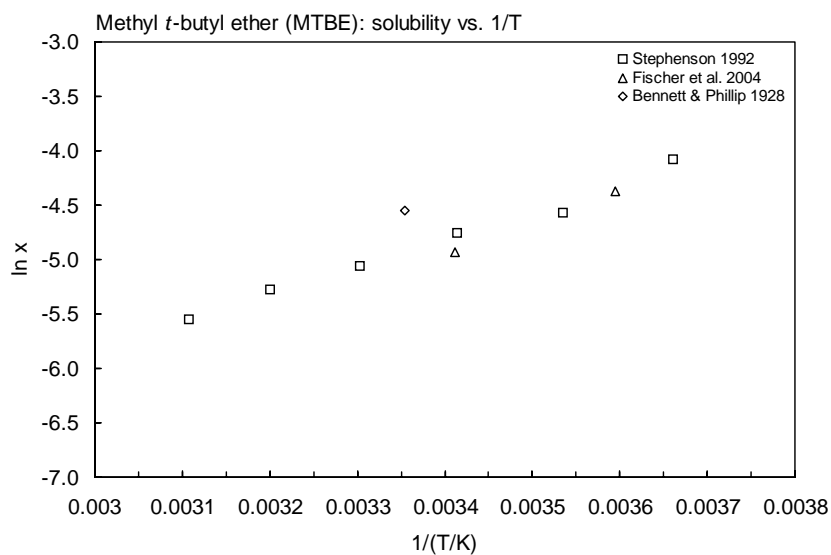


FIGURE 10.1.1.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

TABLE 10.1.1.3.2

Reported vapor pressures of methyl *tert*-butyl ether (MTBE) at various temperatures

Ambrose et al. 1976				Krähenbühl & Gmehling 1994			
comparative ebulliometry				static method*			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
14.847	21805	73.873	180280	300.956	37417	342.570	158286
18.83	25843	77.828	201818	304.397	42944	342.592	158403
23.243	31156	25	33530	307.896	49188	342.652	158669
27.518	37194			312.707	58733		
32.143	44576	$\log P = A - B/(C + t/^{\circ}\text{C})$		318.586	72841	*complete list see ref.	
37.16	53942		P/mmHg	323.663	86748		
41.525	63351	A	6.09379	323.666	86855		
44.835	71313	B	1173.036	328.498	102046		
51.182	88805	C	-41.366	328.528	102133		
55.028	100933	bp	328.30 K	333.387	119445		
55.826	103610			333.386	119444		
60.318	119700	coefficients of		338.224	138873		
64.376	135835	also given in text		338.229	138893		
69.193	157164			338.232	138905		

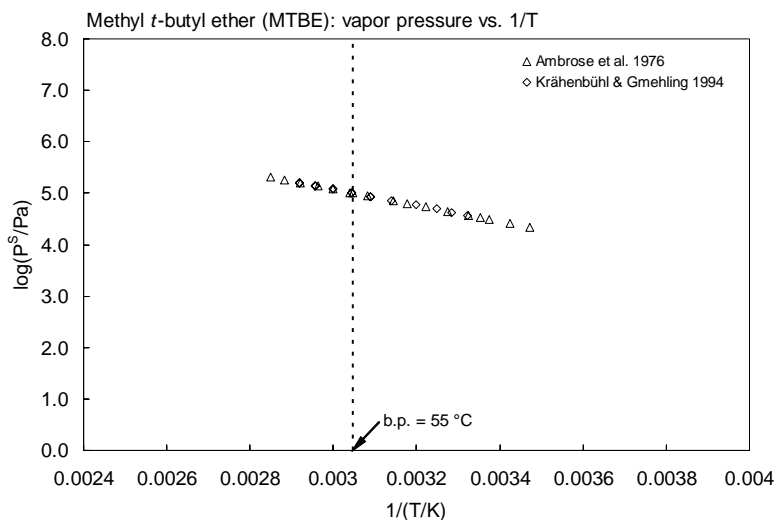
FIGURE 10.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

TABLE 10.1.1.3.3
Reported Henry's law constants of methyl *tert*-butyl ether (MTBE) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Robbins 1993		Bierwagen & Keller 2001		Fischer et al. 2004	
static headspace-GC		SPME-GC		equilibrium concn ratio-GC	
<i>t</i> /°C	H/(Pa m ³ /mol)	<i>t</i> /°C	H/(Pa m ³ /mol)	<i>t</i> /°C	H/(Pa m ³ /mol)
25	53.5	15	93.2	3	20.9
30	120.6	25	137.6	5	25.9
40	223.9	30	179.2	10	27.5
45	367.8	40	222.0	15	42.4
50	413.4			20	54.6
				25	72.4
eq. 1	H/(atm m ³ /mol)	eq. 1a	K _{AW}		
A	18.4	A	6.6475		
B	7666	B	3178		

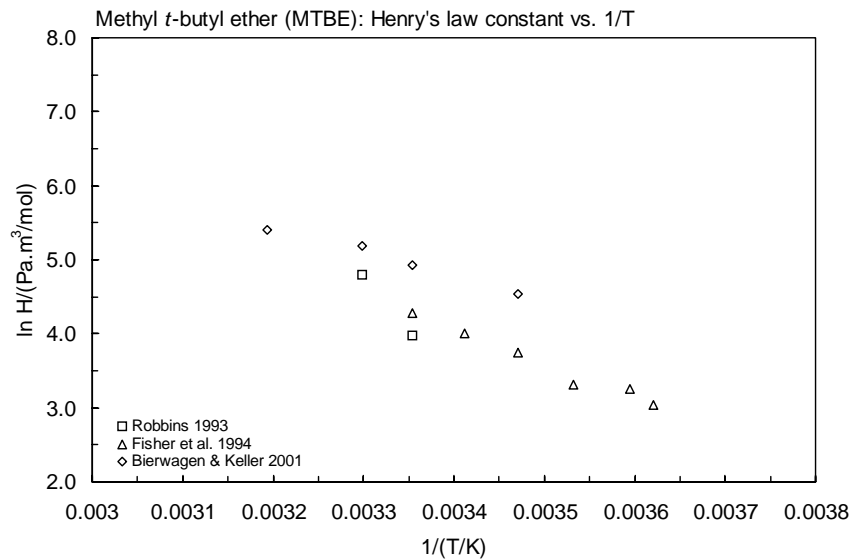
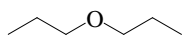


FIGURE 10.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for methyl *t*-butyl ether (MTBE).

10.1.1.4 Di-*n*-propyl ether

Common Name: Di-*n*-propyl ether

Synonym: 4-oxaheptane, 1,1'-oxibispropane, 1-propoxypropane, propyl ether

Chemical Name: di-*n*-propyl ether, propyl ether, 4-oxaheptane

CAS Registry No: 111-43-3

Molecular Formula: C₆H₁₄O, (*n*-C₃H₇)₂O

Molecular Weight: 102.174

Melting Point (°C):

−114.8 (Lide 2003)

Boiling Point (°C):

90.08 (Riddick et al. 1986; Lide 2003)

Density (g/cm³ at 20°C):

0.7466, 0.7419 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

136.9 (20°C, calculated-density)

151.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.78 (quoted, Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4900* (thermostatic volumetric method, measured range 0–25°C, Bennett & Phillip 1928)

2500* (synthetic method, measured range 0–25°C, Bennett & Phillip 1928)

3000 (Seidell 1941; Lange 1971)

2508 (selected, Hine & Mookerjee 1975)

4900 (selected, Riddick et al. 1986)

3820 (literature data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

9072* (calculated-Antoine eq. regression, temp range −43.3 to 89.5°C, Stull 1947)

16358* (39.703°C, comparative ebulliometry, measured range 39.703–98.183°C, Meyer & Hotz 1973)

log (P/mmHg) = [−0.2185 × 8229.6/(T/K)] + 7.863332; temp range −43.3 to 89.5°C (Antoine eq., Weast 1972–73)

9041* (26.59°C, ebulliometry, measured range 26.59–88.65°C, Cidlinski & Polak 1969; quoted, Boublik et al. 1984)

log (P/cmHg) = 5.894812 − 1227.468/(215.7007 + t/°C); temp range 39.7–98.2°C (comparative ebulliometry, Meyer & Hotz 1973)

7621* (23.174°C, ebulliometry, measured range 292.974–387.883 K, Ambrose et al. 1976)

log (P/kPa) = 6.03075 − 1233.148/{(T/K) + 56.708}; temp range 293–388 K (Antoine eq., ebulliometry, Ambrose et al. 1976)

8378, 8320 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.06887 − 1254.429/(218.781 + t/°C); temp range 26.59–88.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.01902 − 1227.068/(215.654 + t/°C); temp range 39.7–86.18°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.9476 − 1256.5/(219.0 + t/°C); temp range 26–89°C (Antoine eq., Dean 1985, 1992)

8334 (selected, Riddick et al. 1986)

log (P/kPa) = 6.03075 − 1133.748/(216.442 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

8334 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.019715 - 1227.468/(-57.449 + T/\text{K})$; temp range 312–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.0361 - 1236.828/(-56.358 + T/\text{K})$; temp range 292–389 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.50879 - 1579.466/(-12.142 + T/\text{K})$; temp range 385–467 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 8.20381 - 3494.323/(209.259 + T/\text{K})$; temp range 465–510 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 44.0232 - 3.282 \times 10^3/(T/\text{K}) - 12.792 \cdot \log (T/\text{K}) + 1.2682 \times 10^{-10} \cdot (T/\text{K}) + 4.8776 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 150–531 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

350.1 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

175.5, 594.6 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

223.3 (computer value, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.03 (shake flask, Hansch et al. 1968; Leo et al. 1971)

2.03 (recommended, Sangster 1989)

2.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C :

2.97 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate, Lloyd et al. 1976)

$k_{OH}(\text{calc}) = 2.05 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{calc}) = 1.57 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 1.68 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (18.0 \pm 2.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (relative rate method, Bennett & Kerr 1989)

$k_{OH}^* = 1.72 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = (19.9 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (20.3 \pm 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air) for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.1.4.1

Reported aqueous solubilities of di-*n*-propyl ether at various temperatures

Bennett & Phillip 1928			
volumetric method		synthetic method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	10500	0	5800
10	7100	10	4100
15	6100	15	3800
20	5400	20	3000
25	4900	25	2500

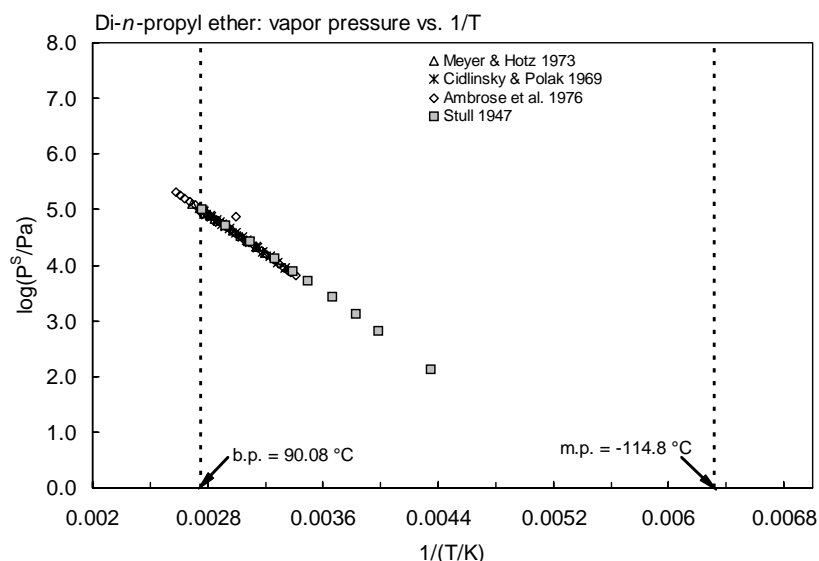
FIGURE 10.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-propyl ether.

TABLE 10.1.1.4.2

Reported vapor pressures of di-*n*-propyl ether at various temperatures and the coefficients for the vapor pressure equations

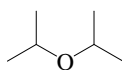
log P = A – B/(T/K)	(1)	ln P = A – B/(T/K)	(1a)
log P = A – B/(C + t/°C)	(2)	ln P = A – B/(C + t/°C)	(2a)
log P = A – B/(C + T/K)	(3)		
log P = A – B/(T/K) – C·log (T/K)	(4)		
log P = A = [1 – T _B /T]	(5)	where log A = (a + bT + CT ²)	

Stull 1947		Meyer & Hotz 1973		Cidlinsky & Polak 1969		Ambrose et al. 1976	
summary of literature data		comparative ebulliometry		Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–43.3	133.3	39.703	16358	26.59	9041	19.824	6442
–22.3	666.6	45.857	21223	31.42	11344	23.174	7621
–11.8	1333	51.773	26.953	36.48	14271	26.887	9130
0	2666	57.749	33962	40.83	17252	30.501	10829
13.2	5333	63.263	41649	45.08	20.662	34.27	12873
21.6	7999	69.298	51617	46	21463	38.124	15283
33	13332	75.199	63121	50.47	25724	41.833	17938

TABLE 10.1.1.4.2 (Continued)

Stull 1947		Meyer & Hotz 1973		Cidlinsky & Polak 1969		Ambrose et al. 1976	
summary of literature data		comparative ebulliometry		Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50.3	26664	77.936	69101	52.94	28338	46.698	21992
69.5	53329	81.601	77811	55.89	31760	50.87	26026
89.5	101325	84.221	84548	60.7	38035	55.827	31341
mp/°C	-112	91.016	104174	65.98	46095	60.296	37380
		98.183	128564	68.76	50822	65.228	44739
		bp/°C	340.096	71.44	55747	70.661	54144
				73.77	60355	75.383	63545
				76.27	65592	60.404	74921
				80.49	76152	85.849	89008
				82.13	79460	90.007	101105
				85.77	83202	95.743	119879
				87.34	93648	100.145	136045
				88.65	97250	105.407	157559
				eq. 2	P/kPa	110.436	180476
						114.733	202031
						25	8334
						eq. 2	P/kPa
				bp/°C	89.952	A	6.03075
						B	1233.748
						C	-56.708
						coefficients of Chebyshev eq.	
						also given in text	

10.1.1.5 Di-isopropyl ether



Common Name: Di-isopropyl ether

Synonym: diisopropoxyde, isopropyl ether, 2-isopropoxypropane, 2,2'-oxybispropane, 3-oxa-2,4-dimethylpentane, IPE, DIPE

Chemical Name: diisopropyl ether, isopropyl ether, 2-isopropoxypropane, 2,2'-oxybispropane, 3-oxa-2,4-dimethylpentane

CAS Registry No: 108-20-3

Molecular Formula: $C_6H_{14}O$, $[(CH_3)_2CH]_2O$

Molecular Weight: 102.174

Melting Point ($^{\circ}C$):

−85.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

68.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7360 (Bennett & Phillip 1928)

0.7239, 0.7185 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

140.0 ($20^{\circ}C$, calculated-density)

151.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.033 (quoted, Riddick et al. 1986)

12.05 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2040 (selected, Hine & Mookerjee 1975)

9000 ($20^{\circ}C$, Verschueren 1983)

12000 ($20^{\circ}C$, selected, Riddick et al. 1986)

11200 (literature data compilation, Yaws et al. 1990)

7900*, 5400 ($20^{\circ}C$, $31^{\circ}C$, shake flask-GC/TC, measured range 0 – $61^{\circ}C$. Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

21410* (calculated-Antoine eq. regression, temp range -57 to $67.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.09712 - 1257.6/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

20093* (temp range 0 – $60^{\circ}C$, Nicolini & Laffitte 1949)

21532* ($26.8^{\circ}C$, ebulliometry, measured range 13.5 – $70.6^{\circ}C$, Flom et al. 1951)

20194* ($25.29^{\circ}C$, ebulliometry, measured range 23.5 – $67.21^{\circ}C$, Cidlinsky & Polak 1969; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 7777.3/(T/K)] + 7.904664$; temp range -57 to $67.5^{\circ}C$ (Antoine eq., Weast 1972–73)

17778* ($22.489^{\circ}C$, ebulliometry, measured 284.779 – $365.122\ K$, Ambrose et al. 1976)

$\log(P/kPa) = 5.97678 - 1143.073/\{(T/K) + 53.810\}$; temp range 284 – $365\ K$ (Antoine eq., ebulliometry, Ambrose et al. 1976)

19954, 20120 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.78384 - 1050.657/(209.511 + t/^{\circ}C)$; temp range 0 – $60^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 5.97081 - 1137.408/(218.516 + t/^{\circ}C)$; temp range 23.5 – $67.21^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.8495 - 1139.34/(218.7 + t/^{\circ}C)$; temp range 23 – $67^{\circ}C$ (Antoine eq., Dean 1985, 1992)

19880 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 5.97678 - 1143.073/(219.340 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
19950, 19890 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.966496 - 1135.034/(-54.92 + T/\text{K})$; temp range 296–342 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.97661 - 1142.985/(-53.82 + T/\text{K})$; temp range 284–365 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.26597 - 1334.298/(-28.271 + T/\text{K})$; temp range 360–440 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 7.13537 - 2140.415/(80.78 + T/\text{K})$; temp range 436–500 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

19862, 10850 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 35.9552 - 2.0276 \times 10^3/(T/\text{K}) - 2.8551 \cdot \log(T/\text{K}) + 2.7662 \times 10^{-4} \cdot (T/\text{K}) - 9.9111 \times 10^{-14} \cdot (T/\text{K})^2$;
temp range 188–500 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

1010 (calculated as $1/K_{\text{AW}}, C_{\text{W}}/C_{\text{A}}$, reported as exptl., Hine & Mookerjee 1975)

483.3, 594.6 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)

175.6 (computer value, Yaws et al. 1991)

208.8 (23°C , batch air stripping-IR, Nielsen et al. 1994)

212.4 (exponential saturator EXPSAT technique, Dohnal & Hovorka 1999)

231 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.52 (shake flask-GC, Funasaki et al. 1985)

1.56 (calculated-fragment const., Hansch & Leo 1979)

1.52 (recommended, Sangster 1989)

1.52 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.66 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = (1.07 \pm 0.20) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy, $k_{\text{OH}} = (1.13 \pm 0.20) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ by relative rate technique (Nelson et al. 1990)

$k_{\text{OH}}^* = (1.08 \pm 0.09) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–400 K (absolute rate, flash photolysis-resonance fluorescence, Wallington et al. 1993)

$k_{\text{OH}} = (9.9 \pm 0.2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $(1.07 \pm 0.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$ at 298 K (relative rate method, Wallington et al. 1993)

$k_{\text{OH}} = 9.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K using both relative (at 295 K) and absolute techniques over 240–440 K (FT-IR spectroscopy, Wallington et al. 1993)

$k_{\text{OH}} = 2.2 \times 10^{-12} \exp[(445 \pm 1450)/(T/\text{K})]$; temp range 240–440 K (Arrhenius eq., FT-IR, Wallington et al. 1993)

$k_{\text{OH}}(\text{calc}) = 33.3 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = 10.2 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.5.1

Reported aqueous solubilities of di-isopropyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	22800
9.7	10200
20	7900
31	5400
40.8	4100
50.7	2800
61	2200

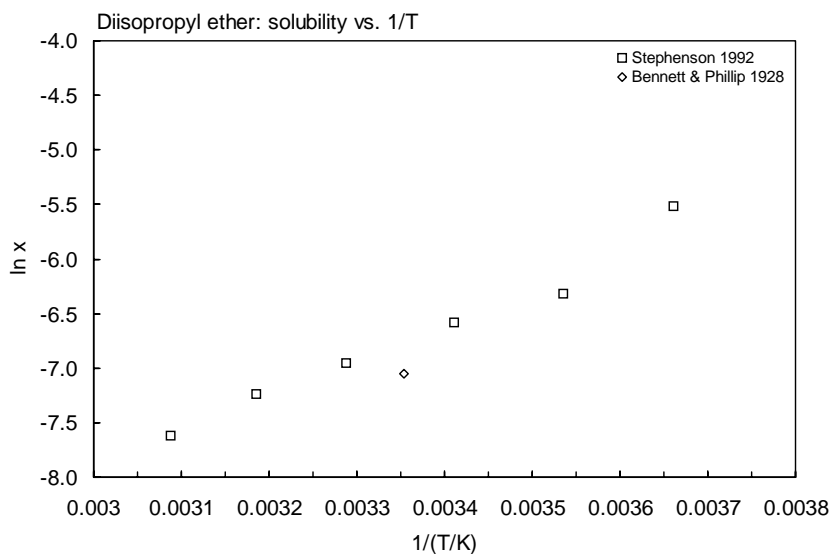


FIGURE 10.1.1.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for di-isopropyl ether.

TABLE 10.1.1.5.2

Reported vapor pressures of di-isopropyl ether at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)				(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)				(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)				(3)					
log P = A – B/(T/K) – C·log (T/K)				(4)					
Stull 1947		Nicolini & Laffitte 1949		Cidlinsky & Polak 1969		Ambrose et al. 1976			
summary of literature data				in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
–57.0	133.3	0	5906	23.5	18654	11.629	10662		
–37.4	666.6	5	7693	25.29	20194	15.253	12712		
–27.4	1333	10	9932	27.42	22177	18.945	15122		
–16.7	2666	15	12679	32	26963	22.489	17778		
–4.50	5333	20	16092	34.22	29591	27.115	21812		
3.4	7999	25	20093	36.93	32980	31.087	25839		
13.7	13332	30	24891	41.17	39005	35.626	31160		
30	26664	35	31651	44.08	43639	40.08	37199		
48.2	53329	40	37530	46.7	48085	44.778	44561		
67.5	101325	45	45329	48.57	51514	49.953	53861		
mp/°C	–60.0	50	54382	50.96	56204	54.454	63367		
		55	64821	54.52	63829	59.24	74743		
		60	76727	56.12	67372	64.423	88818		
				58.17	72427	68.397	100951		
Flom et al. 1951				60.68	78891	69.209	103576		
		dynamic-ebulliometry				63.21	89995	73.855	119720
						64.66	89995	78.057	135878
						65.75	93316	83.078	157382
t/°C	P/Pa					67.21	97.734	87.857	180219
13.5	11466			bp/°C	68.339	91.972	201847		
26.8	21532					25	19880		
35.1	30491			eq. 2	P/kPa				
42.4	40423			A	5.97081	Antoine			
47.9	50356			B	1137.408	eq. 2	P/kPa		
53	60062			C	218.516	A	5.97678		
56.7	68541					B	1143.073		
59.8	76354					C	–53.810		
63	85380					bp/K	341.66		
66.3	95859					coefficients of Chebyshev			
69.5	104205					also given in text.			
70.6	109471								

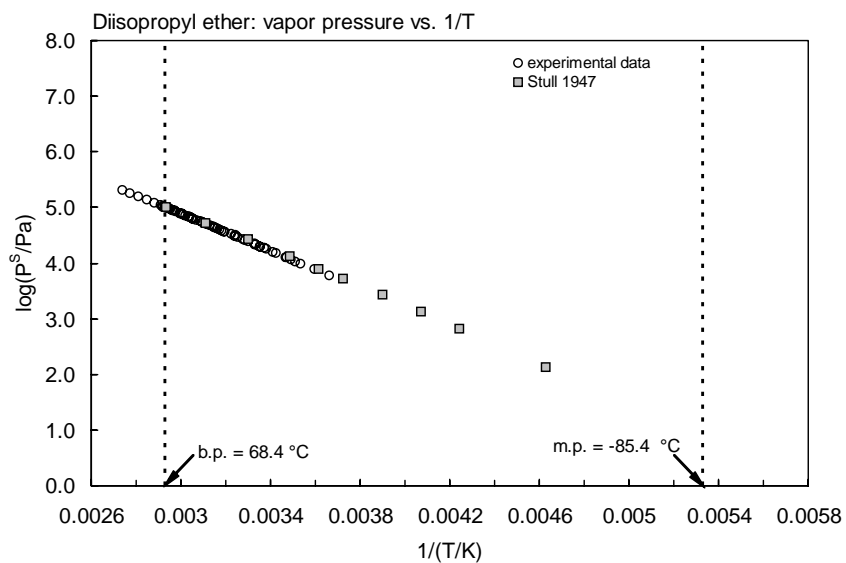
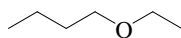


FIGURE 10.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for di-isopropyl ether.

10.1.1.6 Butyl ethyl ether



Common Name: Butyl ethyl ether

Synonym: butyl ethyl ether, 1-ethoxybutane, *n*-butylethyl ether, 3-oxaheptane

Chemical Name: butylethyl ether, 1-ethoxybutane, *n*-butylethyl ether

CAS Registry No: 628-81-9

Molecular Formula: $C_6H_{14}O$, $C_4H_9OCH_2CH_3$

Molecular Weight: 102.174

Melting Point ($^{\circ}C$):

-124 (Lide 2003)

Boiling Point ($^{\circ}C$):

92.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7495, 0.7448 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

136.3 ($20^{\circ}C$, calculated-density)

150.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6500* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.7^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

303164* ($126.67^{\circ}C$, static-Bourdon gauge, measured range 126.67 – $237.78^{\circ}C$, Kobe et al. 1956)

13912* ($38.18^{\circ}C$, ebulliometry, measured range 38.18 – $91.38^{\circ}C$, Cidlinsky & Polak 1969; quoted, Boublik et al. 1984)

$\log(P/kPa) = 6.06257 - 1252.485/(T/K + 56.685)$ (Antoine eq., Ambrose et al. 1976)

9090 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.06565 - 1234.258/(226.668 + t/^{\circ}C)$; temp range 38.18 – $91.38^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.9444 - 1256.4/(216.9 + t/^{\circ}C)$; temp range 38 – $92^{\circ}C$ (Antoine eq., Dean 1985, 1992)

7461 (quoted, Riddick et al. 1986)

$\log(P/kPa) = 6.06257 - 1252.485/(216.465 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

7510 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.062575 - 1252.485/(-56.685 + T/K)$; temp range 311 – $365 K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 8.5224 - 2.4667 \times 10^3/(T/K) + 1.0513 \cdot \log(T/K) - 1.4047 \times 10^{-2} \cdot (T/K) + 9.2664 \times 10^{-6} \cdot (T/K)^2$; temp range 170 – $531 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

136 (calculated-P/C from selected data)

241 (EPICS-static headspace method-GC/FID, Miller & Stuart 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.03 (shake flask-GC, Hansch & Anderson 1967)

2.03 (recommended, Sangster 1989)

2.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.89 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 2.28 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988c)

$k_{OH} = 1.34 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $294 \pm 2 \text{ K}$ (relative rate, Bennett & Kerr 1989)

$k_{OH} = (13.4 - 22.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294–298 K (review, Atkinson 1989)

$k_{OH} = (18.7 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (pulse radiolysis-UV spectroscopy, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.6.1
Reported aqueous solubilities of butyl ethyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	10900
9.3	8300
20	6500
31.2	5300
39.7	5800
50.8	4600
60.2	5100
70.2	3900
80.2	4300
90.7	4000

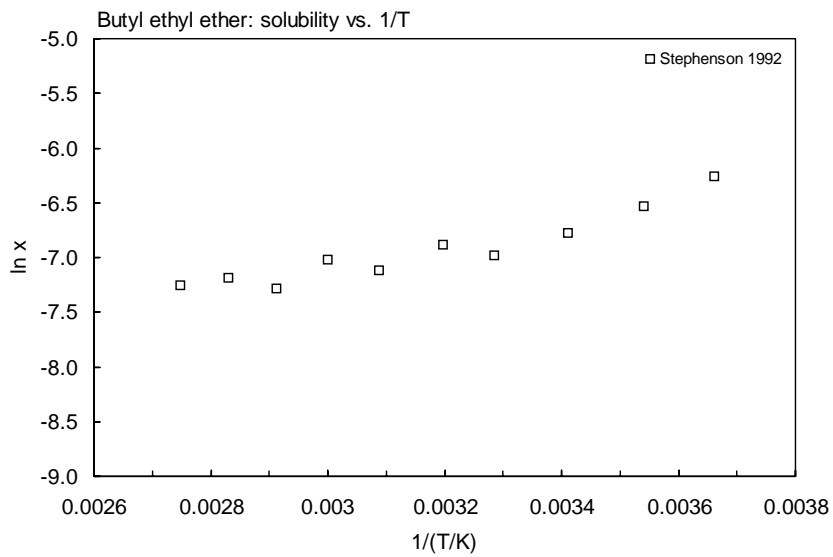


FIGURE 10.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for butyl ethyl ether.

TABLE 10.1.1.6.2
Reported vapor pressures of butyl ethyl ether at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K)$$
$$\log P = A - B/(C + t/^{\circ}\text{C})$$
$$\log P = A - B/(C + T/K)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K)$$

(1)

(2)

(3)

(4)

$$\ln P = A - B/(T/K)$$
$$\ln P = A - B/(C + t/^{\circ}\text{C})$$

(1a)

(2a)

Kobe et al. 1956				Cidlinsky & Polak 1969			
static-Bourdon gauge				in Boublik et al. 1984			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
126.67	303164	204.44	1329789	38.18	13912	79.64	67966
132.22	344505	210	1453811	42.31	16695	82.25	74080
137.78	385846	215.56	1591613	44	17950	85.08	81073
143.33	434076	221.11	1736305	49.04	22146	86.71	85441
148.89	489197	226.67	1894778	52.27	25259	89.73	92885
154.44	544318	232.22	2959149	55.1	28420	91.38	98581
160	613219	237.78	2232392	58.73	32451		
165.56	675230			61.25	35696	bp/°C	92.267
171.11	744131			63.22	38339	Antoine	
176.67	826812			65.85	42271	eq. 2	P/kPa
182.22	909493			68.51	46517	A	6.06565
187.78	1005955			71.66	51925	B	1254.258
193.33	1102416			73.74	55807	C	216.668
198.89	1212658			77.12	62513		

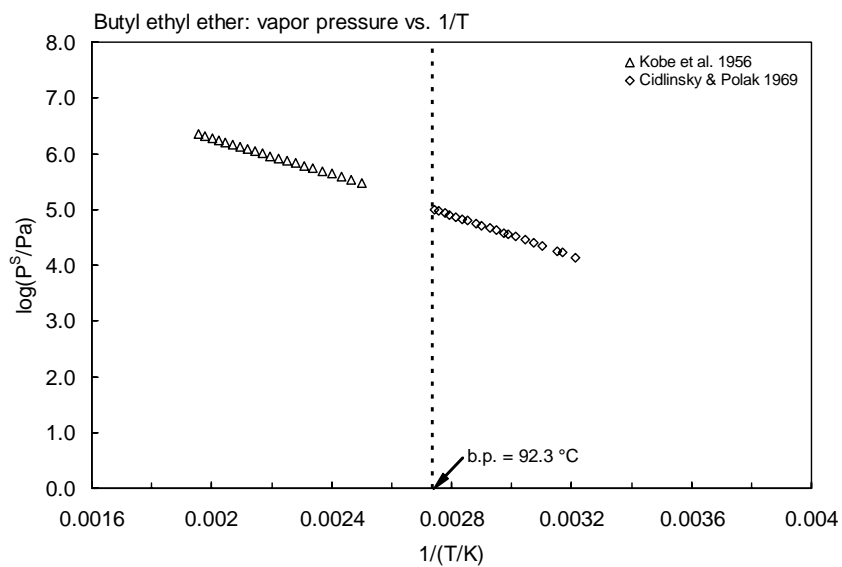
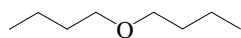


FIGURE 10.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for butyl ethyl ether.

10.1.1.7 Di-*n*-butyl ether

Common Name: Di-*n*-butyl ether

Synonym: 1-butoxybutane, butyl ether, dibutyl ether, *n*-butyl ether, 5-oxanonane, 1,1'-oxybisbutane

Chemical Name: butyl ether, dibutyl ether, di-*n*-butyl ether, *n*-butyl ether, 5-oxanonane, 1,1'-oxybisbutane

CAS Registry No: 142-96-1

Molecular Formula: C₈H₁₈O, (*n*-C₄H₉)₂O

Molecular Weight: 130.228

Melting Point (°C):

−95.2 (Riddick et al. 1986; Lide 2003)

Boiling Point (°C):

140.28 (Lide 2003)

Density (g/cm³ at 20°C):

0.76889, 0.76461 (20°C, 25°C, Dreisbach & Martin 1949)

0.7684, 0.7641 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

170.0 (calculated-density, Wang et al. 1992)

196.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

< 100 (17°C, synthetic method, Bennett & Phillip 1928)

300 (20°C, Verschueren 1983; Riddick et al. 1986)

230* (19.9°C, shake flask-GC/TC, measured range 0–90.6°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7605* (66.84°C, ebulliometry, measured range 67–142°C, Dreisbach & Shrader 1949)

log (P/mmHg) = 7.31540 – 1648.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

80612* (237.78°C, static method-Bourdon gauge, measured range 238–293°C, Kobe et al. 1956)

19529* (89.14°C, ebulliometry, measured range 89.14–140°C, Cidlinsky & Polak 1969)

log (P/kPa) = 5.93018 – 1302.768/(T/K – 81.481); temp range 89–140°C (Cidlinsky & Polak 1969)

log (P/kPa) = 5.93018 – 1302.768/{(T/K) – 81.481} (Antoine eq., ebulliometry, Ambrose et al. 1976)

640 (20°C, Verschueren 1983)

825, 874 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.151 – 1458.718/(141.982 + t/°C); temp range 66.8–141.97°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.92274 – 1298.256/(191.144 + t/°C); temp range 89.14–140.06°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 6.7963 – 1297.3/(191.03 + t/°C); temp range 89–140°C (Antoine eq., Dean 1985, 1992)

898 (select, Riddick et al. 1986)

log (P/kPa) = 5.930185 – 1302.768/(191.669 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

log (P_L/kPa) = 6.4403 – 1648.4/(–42.15 + T/K); temp range 339–415 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.0537 – 1398.8/(–69.55 + T/K); temp range 336–415 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 12.9321 – 3.0416 × 10³/(T/K) + 0.42929 · log (T/K) – 1.237 × 10^{–2} · (T/K) + 7.5943 × 10^{–6} · (T/K)²; temp range 178–581 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

- 608.5 (calculated-1/K_{AW}, C_W/C_A, reported as exptl., Hine & Mookerjee 1975)
 350, 1362 (calculated-group contribution calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW}:

- 3.08 (calculated-f const., Hansch & Leo 1979)
 3.21 (shake flask-GC, Funasaki et al. 1984)
 3.21 (recommended, Sangster 1989)
 3.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA}:

- 3.89 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Volatilization:

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO₃} with NO₃ radical and k_{O₃} with O₃ or as indicated, *data at other temperatures see reference:

k_{OH} = (27.8 ± 3.6) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

k_{OH} = 17 × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 294 ± 2 K (relative rate method, Bennett & Kerr 1989)

k_{OH} = (17.0 – 27.8) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ at 294–298 K (review, Atkinson 1989)

k_{OH} = (27.2 ± 0.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by pulse radiolysis-UV spectroscopy; k_{OH} = (28.8 ± 1.2) × 10⁻¹² cm³ molecule⁻¹ s⁻¹ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k₁) and Elimination (k₂) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance t_{1/2} < 0.24 h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.1.7.1
Reported aqueous solubilities of di-*n*-butyl ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
t/°C	S/g·m ⁻³
0	400
9.3	320
19.9	230
30.9	230
40.3	200
50.3	220
61.3	120
70.5	150
80.7	90
90.5	100

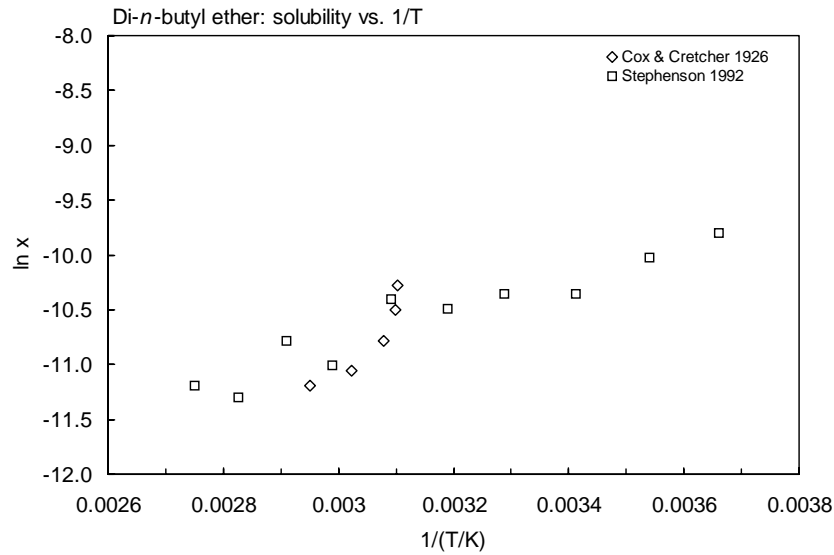


FIGURE 10.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for di-*n*-butyl ether.

TABLE 10.1.1.7.2
Reported vapor pressures of di-*n*-butyl ether at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log (P/mmHg) = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log (P/Pa) = A – B/(C + T/K)		(3)					
log (P/mmHg) = A – B/(T/K) – C.log (T/K)		(4)					
Dreisbach & Shrader 1949		Kobe et al. 1956		Cidlinsky & Polak 1969			
ebulliometry		static method-Bourdon gauge		in Boublik et al. 1984			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
66.84	7605	237.78	806142	89.14	19529	129.67	75155
73.6	10114	243.33	895713	94.57	23957	132.04	80429
85.75	16500	248.89	978394	106.43	36288	134.24	85661
112.28	42066	254.44	1061075	110.54	41580	136.13	90298
127.73	67661	260	1143757	113.28	45509	137.72	94456
141.97	101325	265.56	1247108	114.85	47781	140.06	100666
		271.11	1357350	118.2	53253		
		276.67	1474481	121.05	58118	bp/°C	140.295
		282.22	1598503	123.18	62051	eq. 2	P/kPa
		287.78	1729415	123.41	62509	A	5.92274
		293.33	1874107	125.27	66052	B	1298.256
				127.67	70427	C	191.144

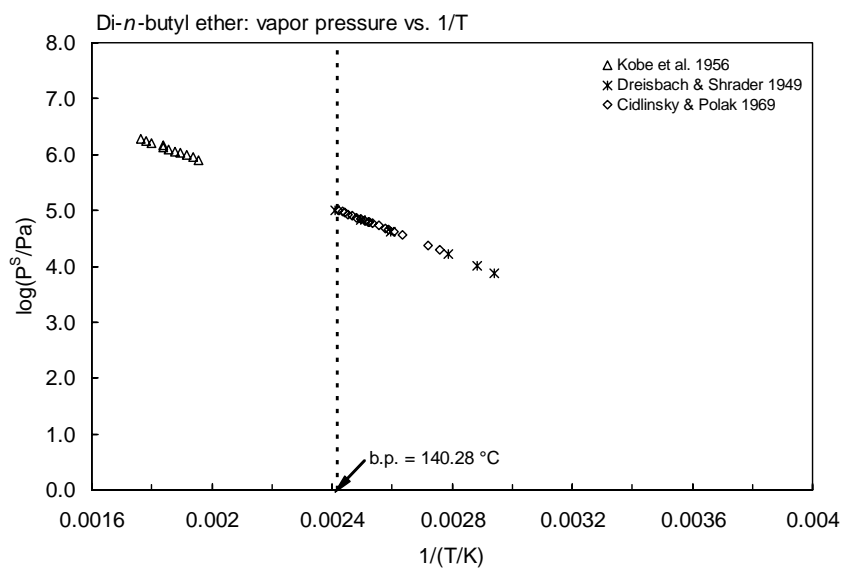


FIGURE 10.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-butyl ether.

10.1.1.8 1,2-Propylene oxide

Common Name: 1,2-Propylene oxide

Synonym: 1,2-epoxypropane, methyloxirane, propylene oxide

Chemical Name: 1,2-propylene oxide, 1,2-epoxypropane, propylene oxide

CAS Registry No: 75-56-9

Molecular Formula: C_3H_6O

Molecular Weight: 58.079

Melting Point ($^{\circ}C$):

-111.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

35 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.859 ($0^{\circ}C$, Verschuereen 1983)

Molar Volume (cm^3/mol):

69.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

6.57, 6.53 (exptl., Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

476000 (US EPA 1981; quoted, Howard 1989)

405000, 650000 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

259000 (literature data compilation, Yaws et al. 1990)

139320 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

74520* (calculated-Antoine eq. regression, temp range -75 to $34.5^{\circ}C$, Stull 1947)

530538* ($87.78^{\circ}C$, static method, measured range 88 – $204^{\circ}C$, Kobe et al. 1956)

51969* ($17.05^{\circ}C$, ebulliometry, measured range -24.17 to $34.75^{\circ}C$ (McDonald et al. 1959)

$\log(P/mmHg) = 6.96997 - 1065.27/(226.283 + t/^{\circ}C)$; temp range -24.17 to $34.75^{\circ}C$ (ebulliometry, McDonald et al. 1959)

70112* (interpolated-Antoine eq., static method, measured range 19.0 – $71.8^{\circ}C$ Bott & Sadler 1966)

$\log(P/mmHg) = 7.658 - 1472/(T/K)$; temp range 19.0 – $71.8^{\circ}C$ (Antoine eq., static method, Bott & Sadler 1966)

$\log(P/mmHg) = [-0.2185 \times 7295.8/(T/K)] + 8.093473$; temp range -75 to $34.5^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = 7.06492 - 1113.6/(232.0 + t/^{\circ}C)$; temp range -35 to $130^{\circ}C$ (Antoine eq., Dean 1985, 1992)

59300, 75900 (20 , $25^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 6.09487 - 1065.27/(226.283 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

71700 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.09487 - 1065.27/(-46.867 + T/K)$; temp range 225 – 308 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 38.5381 - 2.631 \times 10^3/(T/K) - 11.104 \cdot \log(T/K) + 4.2178 \times 10^{-10} \cdot (T/K) + 5.5025 \times 10^{-6} \cdot (T/K)^2$; temp range 161 – 482 K (vapor pressure eq., Yaws 1994)

$\log(P/kPa) = 6.14068 - 1086.37/[(T/K) - 44.556]$; temp range not specified (Antoine eq., Horstmann et al. 2004)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

8.653 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.03 (shake flask, Hansch & Leo 1985, 1987)

0.03	(recommended, Sangster 1989)
0.03	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

−0.20, −0.40 (calculated, Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

0.623	(estimated-S, Lyman et al. 1982; quoted, Howard 1989)
1.477	(calculated-QSAR, Sabljic 1984; quoted, Howard 1989)

Environmental Fate Rate Constants, k , and Half-Lives,:

Volatilization: $t_{1/2}(\text{calc}) \sim 3$ and 18 d from a representative or natural river and oligotrophic lake, respectively (USEPA 1986; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH}(\text{exptl}) = 5.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for gas phase reactions;
 $k = 2.4 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ for the reaction with photochemically produced OH radical in water at room temp. (Güesten et al. 1981; quoted, Howard 1989)

photooxidation $t_{1/2} = 19.3$ d can be calculated for the gas phase reaction with OH radical in air by using Güesten 1981 data and assuming an average OH radical concn. of 8×10^5 molecules/cm³ (GEMS 1986; quoted, Howard 1989)

$k_{OH} = (1.11 \pm 0.75) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to *n*-butane for the gas phase reaction with OH radical in air at $(23.1 \pm 1.1)^\circ\text{C}$ with an atmospheric lifetime of 10 d for an average concentration of 1×10^6 molecules/cm³ of OH radical (Edney et al. 1986)

$k_{OH}(\text{calc}) = 5.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k_{OH}(\text{exptl}) = 5.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{OH} = (4.95 \pm 0.52) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 4.95 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 4.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

Hydrolysis: estimated $t_{1/2} \sim 11.6$ d in fresh water at pH 7 to 9 and $t_{1/2} = 6.6$ d at pH 5 (Howard 1989).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

atmospheric lifetime of 10 d (Edney et al. 1986);

$t_{1/2} = 19.3$ d, based on estimated photooxidation half-life in air by using Güesten et al. 1981 data and assuming an average OH radical concn. of 8×10^5 molecules/cm³ (GEMS 1986; quoted, Howard 1989).

Surface water: calculated $t_{1/2} = 9.15$ yr in natural water by using Güesten et al. 1981 data and assuming an average OH radical concentration of 1×10^{-17} M in natural water (Howard 1989).

Ground water:

Sediment:

Soil:

Biota:

TABLE 10.1.1.8.1

Reported vapor pressures of 1,2-propylene oxide at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log (P/mmHg) = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log (P/Pa) = A – B/(C + T/K)		(3)					
log (P/mmHg) = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Kobe et al. 1956		McDonald et al. 1959		Bott & Sadler 1966	
summary of lit. data		static-Bourdon gauge		ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–75.0	133	87.78	530538	–24.7	6665	19	55462
–57.8	666.6	93.33	599439	–13.66	12170	27	76527
–49.0	1333	98.89	675230	0.77	25345	36.3	107457
–39.8	2666	104.44	771691	17.05	51969	40.8	126656
–28.4	5333	110	868153	33.11	97379	46.8	154253
–21.3	7999	115.56	978394	34.75	103298	50.2	168652
–12.0	13332	121.11	1102416			54	193583
2.1	26664	126.67	1226438			59.2	225847
17.8	53329	132.22	1378020	eq. 2	P/mmHg	64.7	265844
34.5	101325	137.78	1536492	A	6.96997	71.8	320373
		143.33	1701855	B	1065.27		
mp/°C	–112.1	148.89	1880997	C	233.386	eq. 1	P/mmHg
		154.44	2073920			A	7.658
		160	2273733	mp/°C	–112.13	B	1472
		165.56	2506996				
		171.11	2762930				
		176.67	3017864				
		182.22	3300358				
		187.78	3589742				
		193.33	3906687				
		198.89	4251192				
		204.44	4602587				

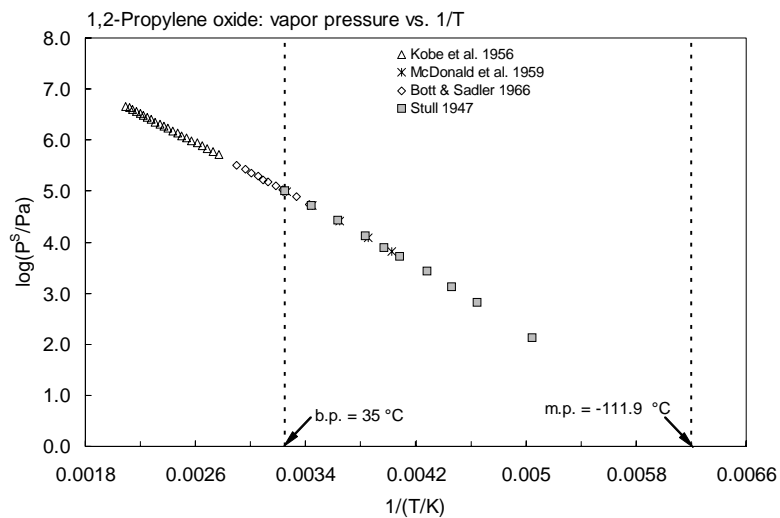


FIGURE 10.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 1,2-propylene oxide.

10.1.1.9 Furan



Common Name: Furan

Synonym: 1,4-epoxy-1,3-butadiene, divinylene oxide, furfuran, oxole, tetrole

Chemical Name: 1,4-epoxy-1,3-butadiene, divinylene oxide, furan

CAS Registry No: 110-00-9

Molecular Formula: C_4H_4O

Molecular Weight: 68.074

Melting Point ($^{\circ}C$):

−85.61 (Lide 2003)

Boiling Point ($^{\circ}C$):

31.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9378 (Dreisbach 1955; Riddick et al. 1986)

0.9514 (Weast 1982–83)

Molar Volume (cm^3/mol):

72.6 ($20^{\circ}C$, calculated-density)

73.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

3.803 (Riddick et al. 1986)

2.05, 3.80 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

10070 (literature average, Valvani et al. 1981)

10000 (Verschueren 1983)

10000 (Riddick et al. 1986)

9900 (literature data compilation, Yaws et al. 1990)

26500 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

70109* ($21.614^{\circ}C$, comparative ebulliometry, measured range $2,552$ – $61.43^{\circ}C$, Guthrie et al. 1952)

$\log(P/mmHg) = 6.97523 - 1060.851/(t/^{\circ}C + 227.740)$; temp range 2.5 – $61.43^{\circ}C$ (Antoine eq., comparative ebulliometry, Guthrie et al. 1952)

79980 (calculated from determined data, Dreisbach 1955)

$\log(P/mmHg) = 6.97523 - 1060.851/(227.740 + t/^{\circ}C)$; temp range -35 to $90^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

627000* ($93.33^{\circ}C$, static-Bourdon gauge, measured range 93.33 – $210^{\circ}C$, Kobe et al. 1956)

$\log(P/mmHg) = [1 - 304.367/(T/K)] \times 10^{0.858337 - 8.56435 \times 10^{-4} \cdot (T/K) + 9.32123 \times 10^{-7} \cdot (T/K)^2}$; temp range 340.95 – 463.65 K (Cox eq., Chao et al. 1983)

70110 ($21.61^{\circ}C$, quoted, Boublik et al. 1984)

79930 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.10017 - 1060.871/(227.742 + t/^{\circ}C)$; temp range: $2,552$ – $61.43^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.97527 - 1060.87/(227.74 + t/^{\circ}C)$; temp range: 2 – $61^{\circ}C$ (Antoine eq., Dean 1985, 1992)

84530 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.10013 - 1060.851/(227.74 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

79930 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.10013 - 1060.851/(-45.41 + T/K)$; temp range 238 – 363 K (Antoine eq., Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 24.9555 - 2.1624 \times 10^3/(T/K) - 6.1066 \cdot \log (T/K) - 2.4185 \times 10^{-10} \cdot (T/K) + 2.0858 \times 10^{-6} \cdot (T/K)^2;$$

temp range 188–490 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

575.5	(calculated-P/C using Riddick et al. 1986 data)
545.8	(computed-vapor liquid equilibrium (VLE) data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.34	(Hansch & Leo 1979;)
1.13	(estimated-HPLC, Garst 1984)
1.14, 1.35	(estimated-MO, π substituent consts., Bodor et al. 1989)
1.34	(recommended, Sangster 1989)
1.34	(recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.50, 1.46; 1.48 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k = 1.4 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ oxidation rate by singlet oxygen in water (Mill 1980; quoted, Mill & Mabey 1985)

$k_{\text{OH}} = (4.01 \pm 0.30) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a atmospheric lifetime $\tau \sim 7 \text{ h}$, $k_{\text{O}_3} = (2.42 \pm 0.28) \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$; and $k_{\text{O}(^3\text{P})} \sim 1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with $\text{O}(^3\text{P})$ atom at 298 K (relative rate method, Atkinson et al. 1983)

$k_{\text{OH}} = (3.98 \pm 0.35) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $22 \pm 2^\circ\text{C}$ (relative rate method, Tuazon et al. 1984)

$k_{\text{OH}}^* = (40.8, 43.1) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 254–424 K (FP-RF flash photolysis-resonance fluorescence, Wine & Thompson 1984)

$k_{\text{O}_3} = 2.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.15 d^{-1} , $k_{\text{OH}} = 4.0 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 3.5 d^{-1} , and $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 29 d^{-1} at room temp. (review, Atkinson & Carter 1984)

$k_{\text{O}_3} = 2.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.15 d^{-1} , $k_{\text{OH}} = 4.0 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 1.7 d^{-1} , and $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 29 d^{-1} at room temp. (review, Atkinson 1985)

$k_{\text{NO}_3} = (1.4 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $295 \pm 2 \text{ K}$ (relative rate method, Atkinson et al. 1985)

$k_{\text{O}_3} = 2.4 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated tropospheric lifetime $\tau = 6.7 \text{ d}$, $k_{\text{OH}} = 4.0 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated $\tau = 6.9 \text{ h}$, and $k_{\text{NO}_3} = 1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated $\tau = 50 \text{ min}$ at room temp. (Atkinson et al. 1985)

$k_{\text{OH}} = 4.07 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson 1987, 1988; quoted, Müller & Klein 1991)

$k_{\text{OH}} = 4.046 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 1.439 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K (Atkinson 1986 and Atkinson et al. 1988, Sabljic & Güsten 1990; Atkinson 1991)

$k_{\text{NO}_3} = 1.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)

$k_{\text{OH}}^* = 4.05 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

calculated atmospheric lifetimes: 6.7 d due to reaction with O_3 in 24-h, 6.9 h due to reaction with OH radical in daytime and 50 min with NO_3 radical at room temp. (Atkinson et al. 1985).

Surface water: $t_{1/2} = 1.0$ h, estimated from oxidation rate by singlet oxygen of $1.4 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ (Mill 1980; quoted, Mill & Mabey 1985).

Ground water:

Sediment:

Soil:

Biota:

TABLE 10.1.1.9.1

Reported vapor pressures of furan at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Guthrie et al. 1952		Kobe et al. 1956					
comparative ebulliometry		static-Bourdon gauge					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
2.552	31160	56.329	232087	93.33	627000	154.44	2156601
7.267	38547	61.43	270110	98.89	709680	160	2370194
12.018	47359			104.44	806142	165.56	1597568
16.797	57803	bp/°C	31.36	110	909493	171.11	2838721
21.614	70109	$\Delta H_v/(kJ\ mol^{-1}) = 27.09$		115.56	1019735	176.67	3107435
26.469	84525		at bp	121.11	1150647	182.22	3389929
31.357	101325			126.67	1295339	187.78	3686204
36.279	120790	eq. 2	P/mmHg	132.22	1440031	193.33	3996258
41.241	143268	A	6.97523	137.78	1605393	198.89	4326983
46.232	169052	B	1060.851	143.33	1770756	204.44	4671488
51.265	198530	C	227.74	149.89	1956788	210	5009103

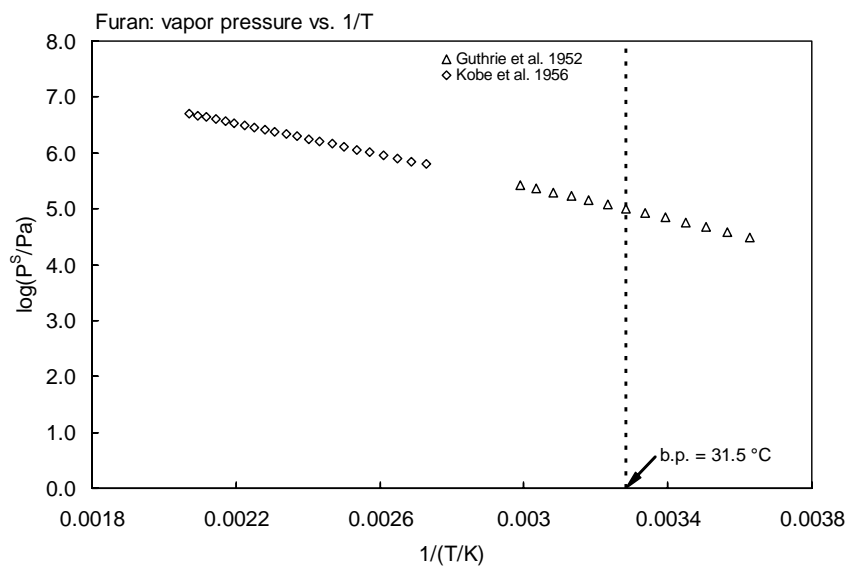


FIGURE 10.1.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for furan.

10.1.1.10 2-Methylfuran



Common Name: 2-Methylfuran

Synonym: silvan, sylvan

Chemical Name: 2-methylfuran

CAS Registry No: 534-22-5

Molecular Formula: C₅H₆O

Molecular Weight: 82.101

Melting Point (°C):

−91.3 (Lide 2003)

Boiling Point (°C):

64.7 (Lide 2003)

Density (g/cm³ at 20°C):

0.913 (Verschuereen 1983)

Molar Volume (cm³/mol):

89.9 (20°C, calculated-density)

95.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

8.66 (exptl., Chickos et al. 1999)

Fugacity Ratio at 25°C, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

3000 (20°C, Verschuereen 1983)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

358285* (110°C, static-Bourdon gauge, measured range 110–254.44°C, Kobe et al. 1956)

86126* (60.3°C, isotenoscope/manometry, measured range 60.3–100.3°C, Eon et al. 1971)

$\log (P/\text{mmHg}) = [1 - 338.704/(T/K)] \times 10^{\{0.871223 - 7.95690 \times 10^{-4} \cdot (T/K) + 7.81737 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 333.45–527.61 K (Cox eq., Chao et al. 1983)

18930, 29990 (20°C, 30°C, quoted, Verschuereen 1983)

23090 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.81244 - 1641.052/(276.164 + t/^\circ\text{C})$; temp range 60.3–100.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

23250 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.95585 - 1107.3/(-56.88 + T/K)$; temp range 251–338 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated):

518 (20°C, calculated-P/C using Verschuereen 1983 data)

Octanol/Water Partition Coefficient, log K_{ow}:

1.85 (shake flask, Log P Database, Hansch & Leo 1987)

1.85 (recommended, Sangster 1989)

1.85 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.1.10.1

Reported vapor pressures of 2-methylfuran at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log(T/K)$	(4)		

Kobe et al. 1956

Eon et al. 1971

static-Bourdon gauge				isoteniscope/manometry			
$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa	$t/^{\circ}C$	P/Pa
110	358285	160	1088636	210	2521777	60.3	86126
115.56	413406	165.56	1205768	215.56	2749150	70.3	119057
121.11	468527	171.11	1329789	221.11	2990303	80.3	161720
126.67	537428	176.67	1467591	226.67	3231457	90.3	215982
132.22	606329	182.22	1612283	232.22	3493281	100.3	283977
137.78	689010	187.78	1770756	237.78	3768885		
143.33	778581	193.33	1943008	243.33	4065159		
149.89	888823	198.89	2122151	248.89	4382104	$\Delta H_v/(kJ\ mol^{-1}) = 30.79$	
154.44	978394	204.44	2321964	254.44	4719719		

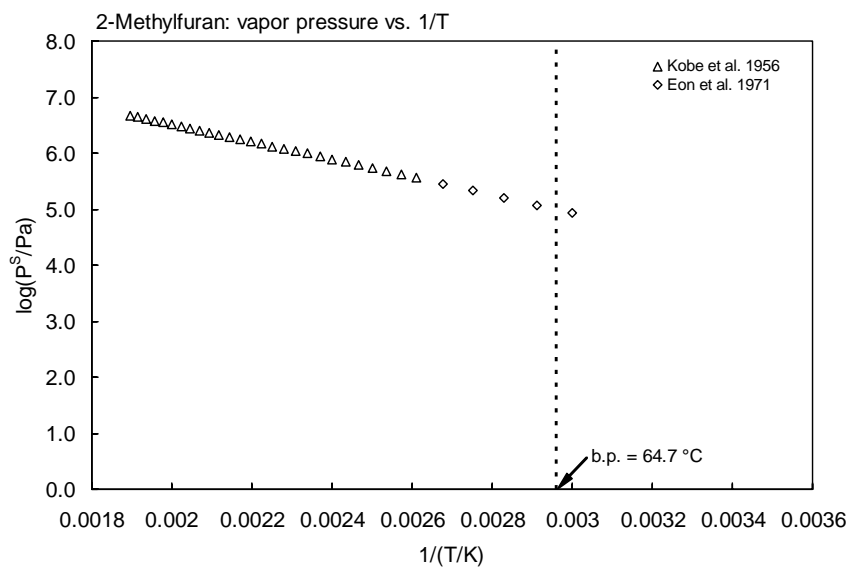


FIGURE 10.1.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for methylfuran.

10.1.1.11 Tetrahydrofuran



Common Name: Tetrahydrofuran

Synonym: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetramethylene oxide

Chemical Name: 1,4-epoxybutane, diethylene oxide, oxacyclopentane, tetrahydrofuran, tetramethylene oxide

CAS Registry No: 109-99-9

Molecular Formula: C_4H_8O

Molecular Weight: 72.106

Melting Point ($^{\circ}C$):

−108.44 (Lide 2003)

Boiling Point ($^{\circ}C$):

65 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8880 (Verschueren 1983)

0.8892 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

81.1 ($20^{\circ}C$, calculated-density)

88.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.535 (quoted, Riddick et al. 1986)

8.54 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Verschueren 1983; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations Additional data at other temperatures designated * are compiled at the end of this section):

23465* (dynamic-ebulliometry, measured 15 – $65^{\circ}C$, Flom et al. 1951)

434076* ($121.11^{\circ}C$, static-Bourdon gauge, measured range 121.11 – $265.56^{\circ}C$, Kobe et al. 1956)

19920* ($23.139^{\circ}C$, measured range 23.2 – $99.7^{\circ}C$, Scott et al. 1970)

21646* (measured range 0.35 – $35^{\circ}C$, Koizumi & Ouchi 1970; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [1 - 339.244/(T/K)] \times 10^4 \{0.830424 - 6.81525 \times 10^{-4} \cdot (T/K) + 6.84786 \times 10^{-7} \cdot (T/K)^2\}$; temp range 253.15 – 540.15 K (Cox eq., Chao et al. 1983)

17530, 26340 ($20^{\circ}C$, $30^{\circ}C$, quoted, Verschueren 1983)

21610, 21630 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.59372 - 1446.15/(249.982 + t/^{\circ}C)$; temp range 0.35 – $35^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.12023 - 1202.394/(226.267 + t/^{\circ}C)$; temp range 23.139 – $99.7^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.97231 - 540.5/(260.10 + t/^{\circ}C)$; temp range not specified (Antoine eq., Dean 1985, 1992)

19920, 21600, 26870 (23.139 , 25 , $30^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 6.79696 - 1157.06/(t/^{\circ}C + 206.75)$, temp range: 90 – $140^{\circ}C$, (Antoine eq., Riddick et al. 1986)

21620, 21900 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.92617 - 1101.47/(-57/95 + T/K)$; temp range 273 – 339 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.12052 - 1202.561/(-46.863 + T/K)$; temp range 296 – 373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.63507 - 1626.656/(15.041 + T/K)$; temp range 399 – 479 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.73137 - 1702.922/(23.613 + T/\text{K})$; temp range 467–541 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 34.870 - 2.7523 \times 10^3/(T/\text{K}) - 9.5958 \cdot \log (T/\text{K}) + 1.9889 \times 10^{-10} \cdot (T/\text{K}) + 3.5465 \times 10^{-6} \cdot (T/\text{K})^2$;
temp range 165–540 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

7.15 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

10.33, 142.6 (calculated-group contribution calculated-bond contribution method, Hine & Mookerjee 1975)

Octanol Water Partition Coefficient, $\log K_{OW}$:

0.46 (calculated-f const., Hansch & Leo 1979)

0.22 (shake flask-GC, Funasaki et al. 1985)

0.46 (shake flask, Log P Database, Hansch & Leo 1987)

0.46 (recommended, Sangster 1989)

0.46 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.86 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.37, 1.26; 1.33 (Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.59 - 1.63) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (FP-RF flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

$k_{OH}(\text{calc}) = 1.66 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(\text{exptl}) = 1.50 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 1.28 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1986, 1987; quoted, Sabljic & Güsten 1990)

$k_{OH}(\text{calc}) = 1.28 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987, 1988; quoted, Müller & Klein 1991)

$k_{NO_3} = 4.875 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Atkinson 1991)

$k_{NO_3} = 4.88 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (relative rate method, Atkinson et al. 1988, Atkinson 1991)

$k_{OH} = 1.78 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 296 K (RP-RF method, Wallington et al. 1988b)

$k_{OH} = 1.61 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}^* = 18.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method; $k_{OH} = 16.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 16 h at $298 \pm 2 \text{ K}$; measured range 263–372 K (Moriarty et al. 2003)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

Surface water:

Ground water:

Sediment:

Soil: disappearance $t_{1/2} = 5.7$ d was calculated from measured first-order rate constant (Anderson et al. 1991).

Biota:

TABLE 10.1.1.11.1

Reported vapor pressures of tetrahydrofuran at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Flom et al. 1951		Kobe et al. 1956		Koizumi & Ouchi 1970		Scott 1970	
dynamic-ebulliometry		static-Bourdon gauge		in Boublik et al. 1984		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
15	15199	121.11	434076	0.35	567	23.139	19920
25	23465	126.67	509867	10	10732	28.362	25007
35	35064	132.22	578768	15	13687	33.62	31160
45	51329	137.78	661450	20	17240	38.917	38547
55	73327	143.33	744131	25	21646	44.251	47359
65	101325	148.89	833702	30	26842	49.62	57803
		154.44	909493	35	35031	55.029	70109
bp/°C	66.1	160	1005955			60.475	84525
		165.56	1116196			65.965	101325
		171.11	1233328			71.489	120.789
		176.67	1364240			77.054	143.268
		182.22	1502042			82.659	169052
		187.78	1653624			88.3	198530
		193.33	1777646			93.98	232087
		198.89	1984349			99.7	270110
		204.44	2156601				
		210	2349524			mp/°C	
		215.56	2549337				
		21.11	2769820				
		226.67	3004084				
		232.22	3252127				
		237.78	3507061				
		243.33	3782655				
		248.89	4078939				
		254.44	4388994				
260	4705938						
265.56	5050443						

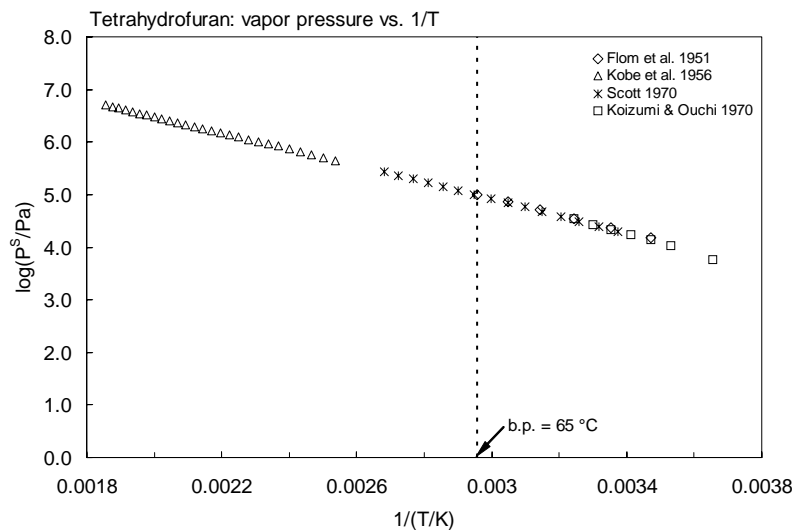


FIGURE 10.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for tetrahydrofuran.

10.1.1.12 Tetrahydropyran



Common Name: Tetrahydropyran

Synonym: pentamethylene oxide, oxacyclohexane

Chemical Name: 1,5-epoxypentane, pentamethylene oxide, oxacyclohexane, tetrahydro-2H-pyran

CAS Registry No: 142-68-7

Molecular Formula: $C_5H_{10}O$

Molecular Weight: 86.132

Melting Point ($^{\circ}C$):

−49.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

88.0 (Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8814, 0.8772 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

97.7 ($20^{\circ}C$, calculated-density)

107.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

80200 (selected, Riddick et al. 1986)

85700*, 68800 ($19.9^{\circ}C$, $31^{\circ}C$, shake flask-GC/TC, measured range $0-81.3^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

9536 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.01171 - 1249.062/(-49.943 + T/K)$; temp range $273-362\ K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

12.71 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

13.94, 215.9 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.64 (shake flask-GC, Funasaki et al. 1985)

0.82 (recommended, Sangster 1989)

1.00 (recommended, Sangster 1993)

0.95 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.22 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} \sim 13.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reactions with OH radical at 298 K (Atkinson 1989)
 $k_{\text{OH}}^* = 11.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method; $k_{\text{OH}} = 12.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 28 h at $298 \pm 2 \text{ K}$, measured range 263–372 K (Moriarty et al. 2003).

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (Darnall et al. 1976);
 photodecomposition $t_{1/2} = 3.4 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976).

TABLE 10.1.1.12.1
Reported aqueous solubilities of tetrahydropyran at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
0	12900
9.4	10030
19.9	8670
31	6880
39.6	6040
50.5	5160
60.7	4620
71.3	4500
81.3	4290

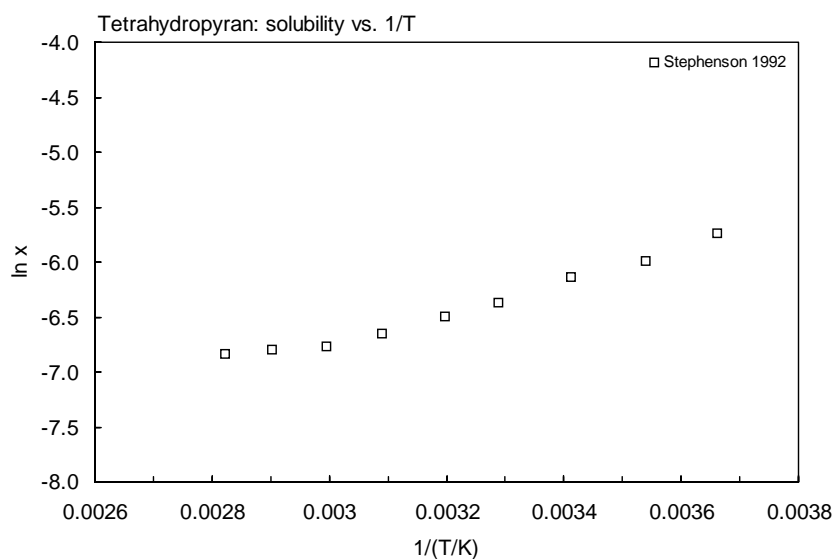


FIGURE 10.1.1.12.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tetrahydropyran.

10.1.1.13 1,4-Dioxane



Common Name: 1,4-Dioxane

Synonym: 1,4-diethylenedioxide, glycolethyleneether, *p*-dioxane

Chemical Name: 1,4-dioxane

CAS Registry No: 123-91-1

Molecular Formula: $C_4H_8O_2$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

11.85 (Lide 2003)

Boiling Point ($^{\circ}C$):

101.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.03318, 1.02766 ($20^{\circ}C$, $25^{\circ}C$, Hovorka et al. 1936)

1.0336, 1.0280 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

85.2 ($20^{\circ}C$, calculated-density)

92.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.46 (quoted, Riddick et al. 1986)

12.84 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Verschueren 1983; Riddick et al. 1986; Howard 1990)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations, *data at other temperatures are tabulated at end of this section):

4920* (static method, measured range 10 – $80^{\circ}C$, Hovorka et al. 1936)

$\log (P/mmHg) = 8.0588 - 1933.8/(T/K)$; temp range 10 – $80^{\circ}C$ (Antoine eq., static method, Hovorka et al. 1936)

$\log (P/mmHg) = 7.8642 - 1866.7/(T/K)$; temp range ~ 10 – $110^{\circ}C$ (Antoine eq., differential manometer, Gallagher & Hibbert 1937)

4986* (static-Hg manometer, measured range 20 – $105^{\circ}C$, Crenshaw et al. 1938; quoted, Vinson & Martin 1963)

$\log (P/mmHg) = -2316.26/(T/K) - 2.77251 \cdot \log (T/K) + 16.2007$; temp range 20 – $105^{\circ}C$ (Hg manometer, Crenshaw et al. 1938)

5333* (summary of literature data, Stull 1947)

406516* ($154.44^{\circ}C$, static-Bourdon gauge, measured range 154.44 – $310^{\circ}C$, Kobe et al. 1956)

$\log (P/mmHg) = [-0.2185 \times 8546.2/(T/K)] + 7.864110$; temp range -35.8 to $101^{\circ}C$ (Antoine eq., isomer not specified, Weast 1972–73)

5065 (Boublik et al. 1984)

4932 (quoted, Verschueren 1983)

$\log (P/kPa) = 6.66014 - 1556.983/(240.366 + t/^{\circ}C)$; temp range 20 – $105^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/kPa) = 6.56891 - 1550.445/(240.459 + t/^{\circ}C)$; temp range 20 – $125^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

4950, 6135 (25 , $30^{\circ}C$, Riddick et al. 1986)

$\log (P/kPa) = 6.9891 - 1866.7/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

4915 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.40318 - 1457.97/(-42.888 + T/\text{K})$; temp range 285–375 K (Antoine eq., Stephenson & Malanowski 1987)

5060, 6092 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 20.5761 - 2.4658 \times 10^3/(T/\text{K}) - 4.3645 \cdot \log (T/\text{K}) - 2.7053 \times 10^{-10} \cdot (T/\text{K}) + 8.5235 \times 10^{-6} (T/\text{K})^2$; temp range 285–587 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated):

0.495 (calculated as $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975; quoted, Howard 1990)

0.431, 1.564 (calculated-group contribution, calculated-bond contribution method Hine & Mookerjee 1975)

0.698 (computer value, Yaws et al. 1991)

1.609, 4.314, 6.925, 10.19 (dioxane, 40, 60, 70, 80°C, equilibrium headspace-GC, Kolb et al. 1992)

$\ln (1/K_{AW}) = -7.940 + 4798/(T/\text{K})$, temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)

0.496 (quoted from Howard 1989–1991, Capel & Larson 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.42, 0.01 (observed, calculated-f const., Chou & Jurs 1979)

−0.42 (quoted, Verschueren 1983; quoted, Pinal et al. 1990)

−0.27 (Hansch & Leo 1985; quoted, Howard 1990; Capel & Larson 1995)

−0.27 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.17 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.23 (soil, estimated- K_{OW} , Lyman et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated Henry' law constant suggests that volatilization for 1,4-dioxane from water and moist soil should be slow; however, it has a moderate vapor pressure, so volatilization from dry soil is possible (Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 67$ d to 9.1 yr in water, based on measured rates for the reaction with hydroxyl radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991)

photooxidation $t_{1/2} = 8.1$ –81 h in air, based on measured rate constant for the reaction of 1,3,5-trioxane with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

photooxidation $t_{1/2} = 6.69$ –9.6 h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radicals (Howard 1990)

$k_{OH} = 10.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 38.6 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 10.9 \times 10^{-12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

$k_{OH}^* = 9.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method; $k_{OH} = 12.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse laser photolysis-laser induced fluorescence and atmospheric lifetime calculated to be 25 h at 298 ± 2 K; measured range 263–372 K (Moriarty et al. 2003)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 672$ –4320 h, based on unacclimated aerobic aqueous screening test data with confirmed resistance to biodegradation (Sasaki 1978; Kawasaki 1980; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688$ –17280 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 28$ d, $t_{1/2}(\text{anaerobic}) = 110$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 8.1\text{--}81$ h, based on estimated photooxidation half-life in air (Atkinson 1987; quoted, Howard et al. 1991);
 $t_{1/2} = 6.69\text{--}9.6$ h in the atmosphere, based on estimated reaction rate with photochemically produced hydroxyl radical (Howard 1990).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

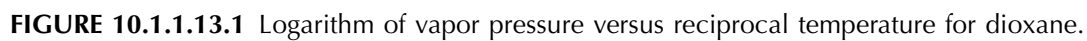
Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 10.1.1.13.1

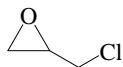
Reported vapor pressures of 1,4-dioxane at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Hovorka et al. 1936		Crenshaw et al. 1938		Stull 1947		Kobe et al. 1956	
static method		ebulliometry-Hg manometer		summary of literature data		static method-Bourdon gauge	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
10	2266	20	3853	–35.8	133.3	154.44	406516
20	3746	25	4986	–12.8	666.6	160	461637
25	4920	30	6386	–1.20	1333	165.56	523648
30	6346	40	10239	12	2666	171.11	585659
40	10212	50	15905	25.2	5333	176.67	654560
50	15972	60	23985	33.8	7999	182.22	730351
60	24171	70	35224	45.1	13332	187.78	806142
70	35583	80	50503	62.3	26664	193.33	902603
80	51036	90	70821	81.8	53329	198.89	992174
		100	97350	101.1	101325	204.44	1095526
eq. 1	P/mmHg	105	113351			210	1205768
A	8.0588			mp/°C	10	215.56	1322899
B	1933.8	bp/°C	101.26			221.11	1440031
						226.67	1577833
		eq. 4	P/mmHg			232.22	1722525
		A	16.2007			237.78	1874107
		B	2316.26			243.33	2039470
		C	2.77251			248.89	2211722
						254.44	2397755
						260	2597568
						265.56	2797381
						271.11	3052314
						276.67	3259017
						282.22	3507061
						287.78	3755105
						293.33	4037599
						298.89	4333873
						204.44	4595697
						310	4933312



10.1.2 HALOGENATED ETHERS

10.1.2.1 Epichlorohydrin



Common Name: Epichlorohydrin

Synonym: 1-chloro-2,3-epoxypropane, (chloromethyl)oxirane, α -epichlorohydrin, γ -chloropropylene oxide

Chemical Name: epichlorohydrin, 1-chloro-2,3-epoxypropane, α -epichlorohydrin, γ -chloropropylene oxide

CAS Registry No: 106-89-8

Molecular Formula: C_3H_5OCl

Molecular Weight: 92.524

Melting Point ($^{\circ}C$):

−57.2 (Riddick et al. 1986; Howard 1989)

−26 (Lide 2003)

Boiling Point ($^{\circ}C$):

118 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1807, 1.1746 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

78.4 ($20^{\circ}C$, calculated-density)

90.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

65800 ($20^{\circ}C$, selected, Riddick et al. 1986)

65800 ($20^{\circ}C$, Krijgsheld & Van der Gen 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2400 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.5958 - 1587.9/(230 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

2192 (Daubert & Danner 1985)

$\log(P_L/kPa) = 6.5958 - 1587.9/(-43.15 + T/K)$; temp range 328–388 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 24.764 - 2.8846 \times 10^3/(T/K) - 5.6252 \cdot \log(T/K) - 1.1011 \times 10^{-10} \cdot (T/K) + 5.3331 \times 10^{-7} \cdot (T/K)^2$; temp range 216–610 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

3.375 (calculated-P/C using Riddick et al. 1986 data)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.30 (Krijgsheld & Van der Gen 1986)

0.45 (shake flask-GC, Deneer et al. 1988)

0.45 (recommended, Sangster 1993)

0.45 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

0.66 (estimated, Santodonato et al. 1980; quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{oc}$:

2.09 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: evaporation $t_{1/2} \sim 29$ h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} \sim 4.0$ d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989)

$k_{OH}(\text{calc}) = 9.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 4.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} \geq 5.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to *n*-butane for the gas phase reaction with OH radical at $23.3 \pm 0.9^\circ\text{C}$ with an atmospheric lifetime of < 21 d for an average OH radical concentration of 1×10^6 molecules/cm³ (Edney et al. 1986)

$k_{OH}(\text{exptl}) = 4.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987)

$k_{O_3}(\text{aq.}) \leq 0.003 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 4.1 and 22°C , with $t_{1/2} \sim 130$ d at pH 7 (Yao & Haag 1991).

Hydrolysis: half-life of 8.2 d in distilled water to hydrolyze to 1-chloropropan-2,3-diol at 20°C and pH 5–9 (Mabey & Mill 1978; quoted, Howard 1989; Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Bridie et al. 1979; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ –2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: photodecomposition $t_{1/2} = 16.0$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976); $t_{1/2} \sim 4.0$ d, based on estimation for the photooxidation with hydroxyl radical in air (Cupitt 1980; quoted, Howard 1989);

$t_{1/2} = 146$ –1458 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991); atmospheric lifetime < 21 d due to reactions with OH radical (Edney et al. 1986).

Surface water: evaporation $t_{1/2} = 29$ h for a model river 1 m deep with a 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1989);

$t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

measured rate constant $k \leq 0.003 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 4.1 and 22°C , with $t_{1/2} \sim 130$ d at pH 7 (Yao & Haag 1991).

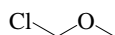
Ground water: 336–1344 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168$ –672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

10.1.2.2 Chloromethyl methyl ether



Common Name: Chloromethyl methyl ether

Synonym: chloromethyl ether, chloromethoxymethane, CMME, monochlorodimethyl ether

Chemical Name: chloromethyl methyl ether

CAS Registry No: 107-30-2

Molecular Formula: C_2H_5ClO , $ClCH_2-O-CH_3$

Molecular Weight: 80.513

Melting Point ($^{\circ}C$):

−103.5 (Verschuereen 1983; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

59.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0703 (Dean 1985)

1.0605 (Budavari 1989)

Molar Volume (cm^3/mol):

75.2 ($20^{\circ}C$, calculated-density)

81.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

decomposes (Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

24900 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.259 - 1240/(-43.15 + T/K)$; temp range 290–332 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 22.7$ – 227 h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $k = 21\ h^{-1}$ at pH 7 and $25^{\circ}C$ with a calculated $t_{1/2} = 2.0$ min (Van Duuren et al. 1972; quoted, Ellington 1989);

$t_{1/2} = 0.0108$ – 0.033 h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991);

hydrolyzed very fast in aqueous solutions with $t_{1/2} < 1.0$ s (Verschuereen 1983).

Biodegradation: aqueous aerobic $t_{1/2} = 168$ – 672 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 672$ – 2688 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 22.7\text{--}227$ h, based on estimated rate constant for the reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

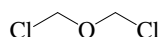
Surface water: $t_{1/2} = 0.0108\text{--}0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Ground water: $t_{1/2} = 0.0108\text{--}0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 0.0108\text{--}0.033$ h, based on measured hydrolysis rate constant for bis(chloromethyl) ether (Tou et al. 1974; quoted, Howard et al. 1991) and chloromethyl methyl ether (Ellington et al. 1987; quoted, Ellington 1989; Howard et al. 1991).

Biota:

10.1.2.3 Bis(chloromethyl)ether

Common Name: Bis(chloromethyl)ether

Synonym: BCME, Bis-CME, chloro(chloromethoxy)methane, dichloromethylether, (dichloro-dimethyl)ether, sym-dichloromethyl ether, oxybis(chloromethane)

Chemical Name: chloromethyl ether, sym-dichloromethyl ether

CAS Registry No: 542-88-1

Molecular Formula: $C_2H_4Cl_2O$, $ClCH_2-O-CH_2Cl$

Molecular Weight: 114.958

Melting Point ($^{\circ}C$):

−41.5 (Weast 1977; Weast 1982–83; Verschueren 1983; Howard 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

106 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.328 ($15^{\circ}C$, Weast 1982–83)

1.315 (Verschueren 1983)

Molar Volume (cm^3/mol):

102.7 (calculated-Le Bas method at normal boiling point)

87.4 (calculated-density, Stephenson & Malanowski 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

22000 (calculated as per Moriguchi 1975 using Quayle 1953 data, Callahan et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

3999 ($22^{\circ}C$, Dreisbach 1952)

$\log(P/mmHg) = -3.4945 - 2.2305 \times 10^3/(T/K) + 6.774 \cdot \log(T/K) - 1.7332 \times 10^{-2} \cdot (T/K) + 9.5511 \times 10^{-6} \cdot (T/K)^2$;
temp range 232–579 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

21.27 (calculated-P/C, Mabey et al. 1982)

21.27 (20 – $25^{\circ}C$ and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

213.18 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

−0.38 (calculated, Radding et al. 1977)

2.40 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

1.041 (bluegill sunfish, Veith et al. 1980)

Sorption Partition Coefficient, $\log K_{oc}$:

1.20 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $k \ll 360 M^{-1} h^{-1}$ for singlet oxygen and $k = 3.0 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982)

photooxidation $t_{1/2} = 0.196$ – 1.96 h, based on estimated rate constant for reaction with hydroxyl radical in air
(Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: hydrolyzed very fast in aqueous solution with half-life in the order of 10 s when extrapolated to pure water (Hammond & Alexander 1972; quoted, Verschueren 1983);
rate constant $k = 0.018 \text{ s}^{-1}$ with $t_{1/2} = 38 \text{ s}$ (Tou et al. 1974; quoted, Callahan et al. 1979; Howard et al. 1991);
hydrolysis $t_{1/2} = 10\text{--}38 \text{ s}$ and will rapidly disappear from any aquatic system (Fishbein 1979; quoted, Howard 1989);

$k = 65 \text{ h}^{-1}$ at pH 7.0 at 20°C (quoted, Mabey et al. 1982).

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}672 \text{ h}$, based on scientific judgement; aqueous anaerobic $t_{1/2} = 672\text{--}2688 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.196\text{--}1.96 \text{ h}$, based on estimated rate constant for reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.0106\text{--}0.106 \text{ h}$, based on estimated hydrolysis half-life in water (Howard et al. 1991).

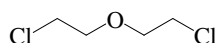
Ground water: $t_{1/2} = 0.0106\text{--}0.106 \text{ h}$, based on estimated hydrolysis in water (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} < 10 \text{ d}$, via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

$t_{1/2} = 0.0106\text{--}0.106 \text{ h}$, based on estimated hydrolysis half-life in water (Howard et al. 1991).

Biota:

10.1.2.4 Bis(2-chloroethyl)ether

Common Name: Bis(2-chloroethyl)ether

Synonym: 2-chloroethyl ether, 1,1'-oxybis(2-chloroethane), bis(β -chloroethyl)ether, Chlorex, 1-chloro-2-(β -chloroethoxy)-ethane, β,β' -dichloroethyl ether, 2,2'-dichloroethyl ether, di(2-chloroethyl)ether, di(chloroethyl)ether, dichlorodiethyl ether, sym-dichlorodiethyl ether

Chemical Name: 2-chloroethyl ether, bis(β -chloroethyl)ether, 1-chloro-2-(β -chloroethoxy)-ethane

CAS Registry No: 111-44-4

Molecular Formula: $C_4H_8Cl_2O$, $ClCH_2CH_2-O-CH_2CH_2Cl$

Molecular Weight: 143.012

Melting Point ($^{\circ}C$):

-51.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

178.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2200 (Verschuereen 1983)

1.2192 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

117.3 ($20^{\circ}C$, calculated-density)

147.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

8.66 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

10200 ($20^{\circ}C$, Du Pont 1966; Verschuereen 1983)

17195 (shake flask-LSC, Veith et al. 1980)

10200 ($20^{\circ}C$, Riddick et al. 1986)

10400*, 10300 ($20^{\circ}C$, $31^{\circ}C$, shake flask-GC/TC, measured range $0-91.7^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

156.2 (Antoine eq. regression, temp range $23.5-178.5^{\circ}C$, Stull 1947)

94.64, 186 (20, $25^{\circ}C$, Verschuereen 1977,1983)

207 (selected, Riddick et al. 1986)

$\log(P/kPa) = 7.2289 - 2359.6/(T/K)$, temp range not specified (Antoine eq., Riddick et al. 1986)

143.6 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.7637 - 1948.62/(-41.974 + T/K)$: temp range $297-452 K$ (Antoine eq., Stephenson & Malanowski 1987)

857.1 (calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

28.97 (calculated-P/C, Lyman et al. 1982; Howard 1989)

1.320 ($20^{\circ}C$, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.58 (calculated, Leo et al. 1971)

1.12 (shake flask-LSC, Veith et al. 1980)

1.29 (shake flask, Hansch & Leo 1985)

1.29 (recommended, Sangster 1993)

1.29 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.041	(bluegill sunfish, Barrows et al. 1980)
1.040	(bluegill sunfish, LSC- ¹⁴ C, Veith et al. 1980; Veith & Kosian 1983)
0.964	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
1.15	(calculated, Sabljic 1987)

Sorption Partition Coefficient, log K_{OC} :

1.38	(soil, calculated-S, Lyman et al. 1982)
1.14	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Volatilization: calculated $t_{1/2} = 5.78$ d (as per Mackay & Wolkoff 1973 by Durkin et al. 1975);

$t_{1/2} = 3.5, 4.4$ and 180.5 d for the streams, rivers and lakes, respectively, were estimated using Henry's law constant (Lyman et al. 1982; quoted, Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 4.0$ h, based on an estimated half-life for ethyl ether in the smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

$k \ll 360 \text{ M}^{-1} \cdot \text{h}^{-1}$ for the reaction with singlet oxygen and $k = 24.0 \text{ M}^{-1} \cdot \text{h}^{-1}$ for the reaction with peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 9.65\text{--}96.5$ h, based on estimated rate constant for the reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: $t_{1/2} = 40.0$ d was estimated at pH 7 from ethyl chloride data in water at an unspecified temperature (Brown et al. 1975; quoted, Howard 1989);

$t_{1/2} = 0.5\text{--}2.0$ yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);

first-order hydrolysis $t_{1/2} = 22$ yr, based on neutral hydrolysis rate constant at 20°C which was extrapolated from data for hydrolysis of dioxane at 100°C (Mabey et al. 1982; quoted, Howard et al. 1991);

$k = 2.6 \times 10^{-5} \text{ h}^{-1}$ at pH 7 and 25°C with a calculated $t_{1/2} = 3.0$ yr (Ellington et al. 1987; quoted, Ellington 1989).

Biodegradation: aqueous aerobic $t_{1/2} = 672\text{--}4320$ h, based on river die-away test data (Ludzack & Ettinger 1963 and Doljido 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 2688\text{--}17280$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $k = 3 \times 10^{-9} \text{ mL cell}^{-1} \cdot \text{h}^{-1}$ for the bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 13.44$ h was estimated for the reaction with OH radical (GEMS 1986; quoted, Howard 1989);

photooxidation $t_{1/2} = 9.65\text{--}96.5$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

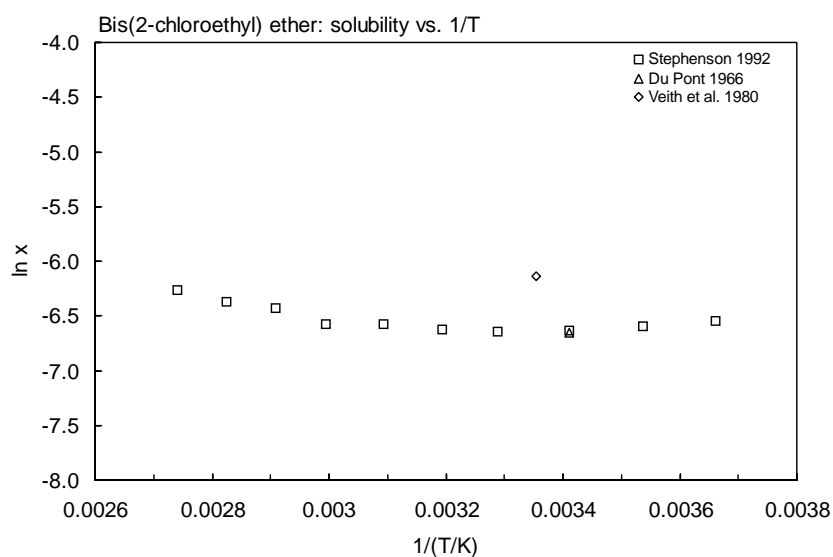
Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

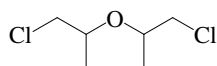
Biota: $t_{1/2} > 4.0$ d but less than 7.0 d in fish tissues (Barrows et al. 1980).

TABLE 10.1.2.4.1**Reported aqueous solubilities of bis(2-chloroethyl) ether at various temperatures**

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	11400
9.6	10900
20	10400
31	10300
40	10500
50.1	11100
60.7	11100
70.6	12800
80.9	13600
91.7	15100

**FIGURE 10.1.2.4.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for bis(2-chloroethyl)ether.

10.1.2.5 Bis(2-chloroisopropyl)ether



Common Name: Bis(2-chloroisopropyl)ether

Synonym: bis(2-chloro-1-methylethyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether, 2,2'-dichloroisopropyl ether, 2,2'-oxybis(1-chloropropane)

Chemical Name: bis(2-chloroisopropyl)ether, dichlorodiisopropyl ether, dichloroisopropyl ether

CAS Registry No: 108-60-1

Molecular Formula: $C_6H_{12}Cl_2O$, $ClCH_2CH(CH_3)-O-CH(CH_3)CH_2Cl$

Molecular Weight: 171.064

Melting Point ($^{\circ}C$):

-97 (Weast 1977; Verschueren 1983)

Boiling Point ($^{\circ}C$):

187 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1100 (Verschueren 1983)

1.1122 (Dean 1985)

Molar Volume (cm^3/mol):

154.1 ($20^{\circ}C$, calculated-density)

193.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1700* (room. temp., Verschueren 1977,1983)

2450*, 2370 ($19.1^{\circ}C$, $31.0^{\circ}C$, shake flask-GC, measured range $9.5-91.4^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

103.95 (Antoine eq. regression, temp range $24.7-180^{\circ}C$, Stull 1947)

113.31 ($20^{\circ}C$, Verschueren 1977,1983)

112.30 ($28.85^{\circ}C$, Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.68233 - 1856.14/(-58.793 + T/K)$; temp range 302–456 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

11.14 ($20^{\circ}C$, calculated-P/C, Mabey et al. 1982)

11.40 (calculated-P/C from Verschueren 1977/83 data)

116.5 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.58 (calculated, Leo et al. 1971)

2.10 (calculated, Mabey et al. 1982)

2.48 (HPLC-RT correlation, Kawamoto & Urano 1989)

2.48 (recommended, Sangster 1993)

Bioconcentration Factor, $\log BCF$:

1.544 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{oc}$:

1.785 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: calculated $t_{1/2} = 1.37$ d (calculated as per Mackay & Wolkoff 1973, Durkin et al. 1975; quoted, Callahan et al. 1979).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 4.0$ h, based on estimated half-life for ethyl ether in a smog chamber (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with singlet oxygen and $k = 2.0 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with peroxy radical (Mabey et al. 1982).

Hydrolysis: $t_{1/2} = 0.5\text{--}2.0$ yr, based on data from chlorinated ethanes and propanes (Dilling et al. 1975; quoted, Callahan et al. 1979);

$k = 4 \times 10^{-6} \text{ h}^{-1}$ at pH 7.0 and 25°C (Mabey et al. 1982).

Biodegradation: aqueous aerobic $t_{1/2} = 432\text{--}4320$ h, based on river die-away test data (Kleopfer & Fairless 1972; quoted, Howard et al. 1991) and aerobic soil column study data (Kincannon & Lin 1985; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 1728\text{--}17280$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: $t_{1/2} = 4.61\text{--}46.1$ h, based on photooxidation half-life in air (Howard et al. 1991).

Surface water: estimated $t_{1/2} = 3.1$ d for surface waters in case of a first order reduction process may be assumed (Zoeteman et al. 1980)

$t_{1/2} = 432\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 864\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 432\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 10.1.2.5.1
Reported aqueous solubilities of bis(2-chloroisopropyl) ether at various temperatures

Stephenson 1992	
shake flask-GC/TC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
9.5	4090
19.1	2450
31	2370
40.3	2180
51.1	1820
60.6	2090
80.7	2650
91.4	2410

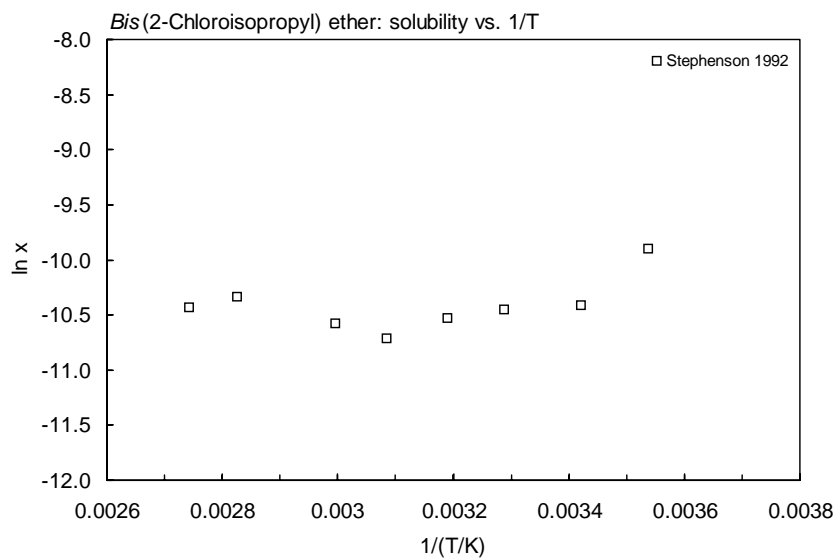
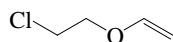


FIGURE 10.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for bis(2-chloroisopropyl)ether.

10.1.2.6 2-Chloroethyl vinyl ether

Common Name: 2-Chloroethyl vinyl ether

Synonym: (2-chloroethoxy)-ethene, β -chloroethyl vinyl ether, vinyl 2-chloroethyl ether

Chemical Name: β -chloroethyl vinyl ether, 2-chloroethyl vinyl ether, vinyl 2-chloroethyl ether

CAS Registry No: 110-75-8

Molecular Formula: $C_4H_7Cl_2O$, $ClCH_2CH_2-O-CH=CH_2$

Molecular Weight: 106.551

Melting Point ($^{\circ}C$):

-70 (Lide 2003)

Boiling Point ($^{\circ}C$):

108 (Weast 1977; Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0475 (Weast 1982–83)

1.0480 (Dean 1985)

Molar Volume (cm^3/mol):

101.7 ($20^{\circ}C$, calculated-density)

119.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

15000 (calculated as per Moriguchi 1975, Callahan et al.)

6000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

3566 ($20^{\circ}C$, calculated, Dreisbach 1952)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$ or as indicated):

0.0253 (20 – $25^{\circ}C$, calculated-P/C, Mabey et al. 1982)

25.33 (20 – $25^{\circ}C$ and low ionic strength, Pankow & Rosen 1988; Pankow 1990)

24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.28 (calculated as per Leo et al. 1971, Callahan et al. 1979)

1.14 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

0.672 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

0.820 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 30$ min, based on half-life estimated for 2-methyl-2-butene from smog chamber data (Altshuller et al. 1962 and Laity et al. 1973; quoted, Callahan et al. 1979);

$k = 1 \times 10^{10} M^{-1} \cdot h^{-1}$ for singlet oxygen and $k = 34 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982).

Hydrolysis: $k = 4.4 \times 10^{-10} s^{-1}$, minimum rate at pH 7 and $25^{\circ}C$ in pure water with a maximum $t_{1/2} = 0.48$ yr (Jones & Wood 1964; quoted, Callahan et al. 1979);

$k \sim 4 \times 10^{-6} h^{-1}$ at pH 7.0 and $25^{\circ}C$ with reference to that of bis(2-chloroethyl)ether (Mabey et al. 1982).

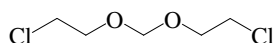
Biodegradation:

Biotransformation: $k = 1 \times 10^{-10} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation to water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Soil: $t_{1/2} < 10 \text{ d}$, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).

10.1.2.7 Bis(2-chloroethoxy)methane

Common Name: Bis(2-chloroethoxy)methane

Synonym: bis(β -chloroethyl)formal, β , β -dichlorodiethyl formal, dichlorodiethyl methylal

Chemical Name: bis(2-chloroethoxy)methane

CAS Registry No: 111-91-1

Molecular Formula: $C_5H_{10}Cl_2O_2$, $ClCH_2CH_2-O-CH_2-O-CH_2CH_2Cl$

Molecular Weight: 173.037

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

215 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

180.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

81000 (calculated as per Moriguchi 1975, Callahan et al. 1979;)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

21.58 (Antoine eq. regression, temp range 53 – $215^{\circ}C$, Stull 1947)

< 13.3 (calculated as per Dreisbach 1952 using data of Webb et al. 1962, Callahan et al. 1979)

21.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.54778 - 2641.33/(-11.518 + T/K)$; temp range 326 – $486\ K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

0.0284 (20 – $25^{\circ}C$, calculated-P/C, Mabey et al. 1982)

0.0273 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.260 (calculated as per Leo et al. 1971, Callahan et al. 1979; Ryan et al. 1988)

1.029 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

0.568 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

0.716 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $k \ll 360\ M^{-1}\ h^{-1}$ for singlet oxygen and $k = 52\ M^{-1}\ h^{-1}$ for peroxy radical (Mabey et al. 1982).

Hydrolysis: minimum rate $k = 2.53 \times 10^{-6}\ L\ mol^{-1}\ s^{-1}$ for acid-catalyzed hydrolysis of the acetal linkage at $25^{\circ}C$ (Kankaanperä 1969; quoted, Callahan et al. 1979; Mabey et al. 1982);

$t_{1/2} = 0.5$ – $2.0\ yr$, based on data of Dilling et al. 1975 on chlorinated ethanes and propanes (quoted, Callahan et al. 1979);

estimated rate constant $k \sim 4 \times 10^{-6}\ h^{-1}$ at pH 7.0 and $25^{\circ}C$ by analogy to bis(2-chloroethyl)ether (Mabey et al. 1982).

Biodegradation:

Biotransformation:

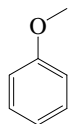
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Soil: $t_{1/2} > 50$ d, via volatilization subject to plant uptake from the soil (Ryan et al. 1988).

10.1.3 AROMATIC ETHERS

10.1.3.1 Anisole (Methoxybenzene)



Common Name: Anisole

Synonym: methoxybenzene

Chemical Name: anisole, methoxybenzene, methyl phenyl ether

CAS Registry No: 100-66-3

Molecular Formula: C_7H_8O , $C_6H_5OCH_3$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

-37.13 (Lide 2003)

Boiling Point ($^{\circ}C$):

153.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.99402, 0.98932 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9940, 0.9893 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

108.8 ($20^{\circ}C$, calculated-density)

127.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1514 (shake flask-UV, McGowan et al. 1966)

1536 (shake flask-UV, Vesala 1974)

2030*, 1860 ($20^{\circ}C$, $29.7^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.7^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

497* (calculated-Antoine eq. regression, temp range 5.4 – $155.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.35950 - 1718.7/(230 + t/^{\circ}C)$ (Antoine eq., temp range 73 – $154^{\circ}C$, Dreisbach & Martin 1949)

6287* ($73.34^{\circ}C$, ebulliometry, measured range 73.34 – $153.75^{\circ}C$, Dreisbach & Shrader 1949)

26547* ($109.876^{\circ}C$, ebulliometry, measured range 109.876 – $164.114^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.05236 - 1489.756/(203.543 + t/^{\circ}C)$; temp range 109.876 – $164.114^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 22.84299 - 3033.20/(T/K) - 4.88720 \cdot \log(T/K)$; temp range 109.876 – $164.114^{\circ}C$ (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = [-0.2185 \times 10440.9/(T/K)] + 8.221443$; temp range 5.4 – $155.5^{\circ}C$ (Antoine eq., Weast 1972–73)

472* (“recomputed” reported data, ebulliometry, measured range 383 – 437 K, Ambrose et al. 1976)

$\log(P/kPa) = 6.17595 - 1489.502/(T/K - 69.577)$; temp range 383 – 437 K (Antoine eq., ebulliometry, Ambrose et al. 1976)

$\log(P/mmHg) = [1 - 426.827/(T/K)] \times 10^{0.942238 - 10.2065 \times 10^{-4} \cdot (T/K) + 10.6819 \times 10^{-7} \cdot (T/K)^2}$; temp range 346.49 – 415.52 K (Cox eq., Chao et al. 1983)

$\log(P/kPa) = 6.23361 - 1529.735/(208.062 + t/^{\circ}C)$; temp range 73.3 – $153.75^{\circ}C$ (Antoine eq. derived from exptl data of Dreisbach & Shrader 1949, Boublik et al. 1984)

$\log(P/kPa) = 6.17900 - 1490.93/(203.675 + t/^{\circ}C)$; temp range 109.9 – $164.1^{\circ}C$ (Antoine eq. derived from reported exptl data of Collerson et al. 1965, Boublik et al. 1984)

- log (P/mmHg) = $7.05269 - 1489.99/(203.57 + t/^{\circ}\text{C})$; temp range 110–164°C (Antoine eq., Dean 1985, 1992)
 472 (selected, Riddick et al. 1986)
 log (P/kPa) = $6.17595 - 1489.502/(203.573 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 log (P_L /kPa) = $6.17622 - 1489.957/(-69.525 + T/\text{K})$; temp range 382–437 K (Antoine eq., Stephenson & Malanowski 1987)
 204, 383 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)
 log (P/mbar) = $7.11773 - 1451.742/[(T/\text{K}) - 73.252]$; temp range 382–429 K (vapor-liquid equilibrium (VLE)-Fischer still, Reich & Sanhueza 1993)
 log (P/mmHg) = $-8.1053 - 2.5386 \times 10^3/(T/\text{K}) + 9.0289 \cdot \log (T/\text{K}) - 2.0426 \times 10^{-2} \cdot (T/\text{K}) + 1.0536 \times 10^{-5} \cdot (T/\text{K})^2$;
 temp range 236–642 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C):

- 430.8 (exptl. $1/K_{AW} = C_W/C_A$, Hine & Mookerjee 1975)
 430.8, 358.3 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, log K_{OW} :

- 2.11 (shake flask-UV, Fujita et al. 1964)
 2.04 (shake flask-UV, Rogers & Cammarata 1969)
 2.10 (HPLC-RT correlation, Mirrlees et al. 1976)
 2.08 (Hansch & Leo 1979)
 2.24 (HPLC- k' correlation, Haky & Young 1984)
 2.16 (HPLC-RT correlation, Ge et al. 1987)
 2.15 (HPLC-RT correlation, Minick et al. 1988)
 2.01 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
 2.11 (recommended, Sangster 1989, 1993)
 2.17 (dual-mode centrifugal partition chromatography, Gluck 1990)
 1.67, 1.79 (shake flask-UV/VIS spec.: 25, 60°C, Kramer & Henze 1990)
 2.11 (recommended, Hansch et al. 1995)
 2.41, 2.31, 2.58, 2.55 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovsaka et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

- 4.01 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 1.34 (Isnard & Lambert 1988)

Sorption Partition Coefficient, log K_{OC} :

- 6.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 1.054 \times 10^{-2} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO- in the gas (Dilling et al. 1988)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.57 \pm 0.24) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K, measured range 299–435 K (overall rate constant, flash photolysis-resonance fluorescence technique, Perry et al. 1977)

$k_{OH} = 1.57 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1985; quoted, Sabljic & Güsten 1990)

$k_{NO_3} = 9.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (re-evaluated value, Atkinson et al. 1987)

$k_{OH} = 1.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air, extrapolated from lit. data to 25°C (Dilling et al. 1988)

$k_{NO_3} = 2.08 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990)

$k_{OH} = (14.1 - 19.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. to 299.9 K (Atkinson 1989)

Hydrolysis:

Biodegradation:

Biotransformation: degradation $k = 2.86 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1}$ in pure culture system (Banerjee et al. 1984).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.3.1.1
Reported aqueous solubilities of anisole at various temperatures

Stephenson 1992

shake flask-GC/TC

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	
10.2	2370
20	2030
29.7	1860
39.9	1840
50.2	1990
60.2	2550
70.2	2530
81.2	2940
90.7	3520

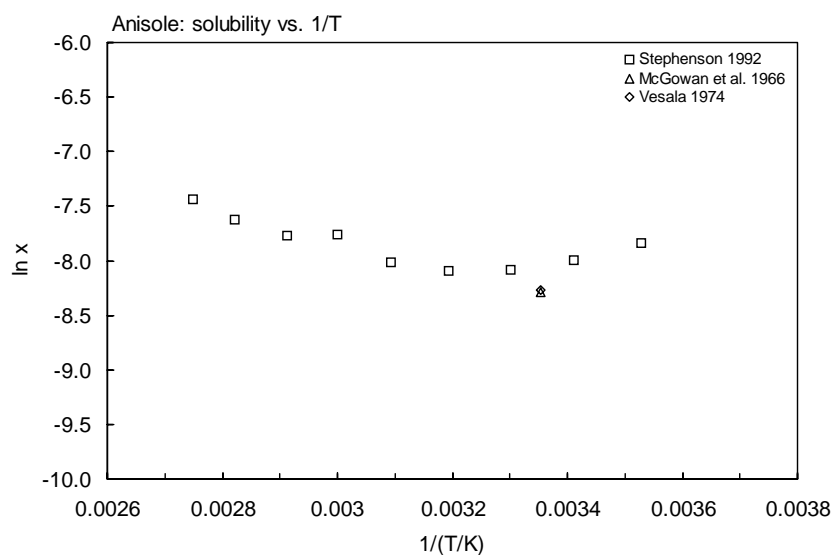


FIGURE 10.1.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for anisole.

TABLE 10.1.3.1.2

Reported vapor pressures of anisole at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
5.4	133.3	73.34	6287	109.876	26547	109.88	26547
30	666.6	81.31	8851	116.255	33024	116.261	33024
42.2	1333	84.55	10114	122.045	39966	122.053	39966
55.8	2666	99.89	16500	126.854	46587	126.864	46587
70.7	5333	123.77	42066	131.266	55425	131.279	53424
80.1	7999	139.37	67661	136.078	59950	135.092	59950
93	13332	153.75	101325	138.64	66614	138.655	66614
112.3	26664			141.919	73266	141.936	73266
133.8	53329			145.003	79992	145.021	79992
155.5	101325	Antoine eq. given by		147.89	86731	147.91	86732
		Dreisbach & Martin 1949		150.429	93021	150.45	93021
mp/°C	–37.3	Eq. 2	P/mmHg	153.143	100135	153.164	100137
		A	7.3595	155.554	106819	155.576	106820
		B	1718.7	157.81	113382	157.834	113381
		C	230	160.009	120086	160.033	120084
				162.087	126698	162.113	126697
		bp/°C	153.75	164.114	133429	164.141	133427
		mp/°C	–37.38			25	472
				bp/°C	153.598		
						Antoine eq.	
				Antoine eq.		eq. 2	P/kPa
				eq. 2	P/mmHg	A	6.17595
				A	705236	B	1489.502
				B	1489.756	C	–69.577
				C	203.543		
				Kirchhoff eq.		Coefficients of Chebyshev eq. are	
				eq. 4	P/mmHg	also given in text.	
				A	22.842 99		
				B	3033.2		
				C	4.8872		
				ΔH _v /(kJ mol ^{–1}) = 39.04			

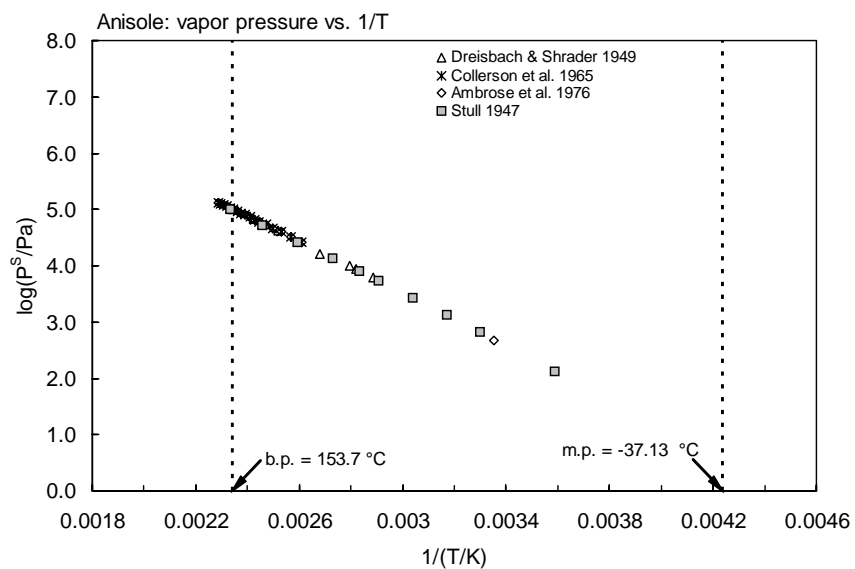
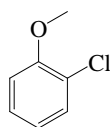


FIGURE 10.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for anisole.

10.1.3.2 2-Chloroanisole



Common Name: 2-Chloroanisole

Synonym: 1-chloro-2-methoxybenzene

Chemical Name: 2-chloroanisole

CAS Registry No: 766-51-8

Molecular Formula: C_7H_7ClO , $C_6H_4Cl(OCH_3)$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$): liquid

−26.8 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

198.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1911 (Lide 2003)

Molar Volume (cm^3/mol):

119.7 ($20^{\circ}C$, calculated-density)

148.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

490 (shake flask-HPLC/UV, Lun et al. 1995)

766 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

6287 ($115.13^{\circ}C$, ebulliometry, measured range 115.13 – $186.19^{\circ}C$, Dreisbach & Shrader 1949)

$\log(P/mmHg) = 7.54073 - 2012.4/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

$\log(P/kPa) = 6.25236 - 1660.008/(189.207 + t/^{\circ}C)$, temp range 115.13 – $186.19^{\circ}C$ (Antoine eq. derived from exptl data of Dreisbach & Shrader 1949, Boublik et al. 1984)

0.0594 (P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.66563 - 2012.4/(-43.15 + T/K)$, temp range 388 – 460 K, (Antoine eq., Stephenson & Malanowski 1987)

0.0302 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

9.50 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.68 (shake flask-UV, Nakagawa et al. 1992)

2.50 (shake flask-HPLC/UV both phases, Lun et al. 1995)

2.72 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

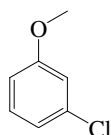
Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.13 (calculated- K_{ow}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

10.1.3.3 3-Chloroanisole



Common Name: 3-Chloroanisole

Synonym:

Chemical Name:

CAS Registry No: 2845-89-8

Molecular Formula: C_7H_7ClO , $C_6H_4Cl(OCH_3)$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

193.5 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

148.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

235 (shake flask-HPLC/UV, Lun et al. 1995)

231 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0282 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

21.4 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.60 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.09 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

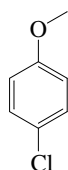
Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.15 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

10.1.3.4 4-Chloroanisole



Common Name: 4-Chloroanisole

Synonym: 1-chloro-4-methoxy-benzene

Chemical Name: 4-chloroanisole

CAS Registry No: 623-12-1

Molecular Formula: C_7H_7ClO , $C_6H_4Cl(OCH_3)$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$):

< -18 (Lide 2003)

Boiling Point ($^{\circ}C$):

197.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.201 (Lide 2003)

Molar Volume (cm^3/mol):

118.7 ($20^{\circ}C$, calculated-density)

148.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

237 (shake flask-HPLC/UV, Lun et al. 1995)

312 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0324 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

18.2 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.78 ($23^{\circ}C$, shake flask-LSC, Banerjee et al. 1980)

2.78 (recommended, Sangster 1993)

2.70 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.00 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.13 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

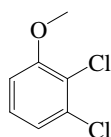
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Biodegradation: degradation rate constants $k = 2.29 \times 10^{-18} mol cell^{-1} h^{-1}$ from pure culture studies (Banerjee et al. 1984).

Half-Lives in the Environment:

10.1.3.5 2,3-Dichloroanisole

Common Name: 2,3-Dichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 1984-59-4

Molecular Formula: $C_7H_6Cl_2O$, $C_6H_3Cl_2(OCH_3)$

Molecular Weight: 177.028

Melting Point ($^{\circ}C$):

32 (Lun et al. 1995; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

169.1 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.854 (mp at $32^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

86.9 (shake flask-GC/ECD, Lun et al. 1995)

140.6 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0468 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

44.1 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.24 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.30 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.05 (calculated- K_{ow}/K_{aw} , Pfeifer et al. 2001)

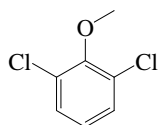
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Half-Lives in the Environment:

10.1.3.6 2,6-Dichloroanisole



Common Name: 2,6-Dichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 1984-65-2

Molecular Formula: $C_7H_6Cl_2O$, $C_6H_3Cl_2(OCH_3)$

Molecular Weight: 177.028

Melting Point ($^{\circ}C$):

10 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

169.1 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

13.12 (shake flask-GC/ECD, Lun et al. 1995)

21.8 (liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0110 (liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

113.7 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

3.14 (shake flask-HPLC/UV both phases, Lun et al. 1995)

3.10 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

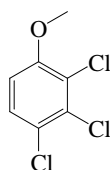
2.53 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.7 2,3,4-Trichloroanisole

Common Name: 2,3,4-Trichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 54135-80-7

Molecular Formula: $C_7H_5Cl_3O$, $C_6H_2Cl_3(OCH_3)$

Molecular Weight: 211.473

Melting Point ($^{\circ}C$):

70 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

190.0 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.362 (mp at $70^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

10.8 (shake flask-GC/ECD, Lun et al. 1995)

22.1 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.263 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

74.7 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.74 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

4.03 (shake flask-GC/ECD, both phases, Lun et al. 1995)

3.92 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.44 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.09 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

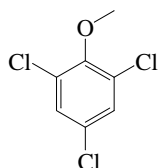
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 1450 mL g^{-1} d^{-1}$; $k_2 = 1.9 d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

10.1.3.8 2,4,6-Trichloroanisole



Common Name: 2,4,6-Trichloroanisole

Synonym:

Chemical Name:

CAS Registry No: 87-40-1

Molecular Formula: $C_7H_5Cl_3O$, $C_6H_2Cl_3(OCH_3)$

Molecular Weight: 211.473

Melting Point ($^{\circ}C$): 61.5 (Lide 2003)

Boiling Point ($^{\circ}C$): 241 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

190.0 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.438 (mp at $61.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

13.2 (shake flask-GC/ECD, Lun et al. 1995)

14.6 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

2.065 (GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0724 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

218.7 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.20 (HPLC-relative retention time correlation, Neilson et al. 1984)

4.11 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

3.96 (reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

4.02 (shake flask-GC/ECD, both phases, Lun et al. 1995)

4.05 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.10 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.90 (zebra fish, Neilson et al. 1984)

2.86 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

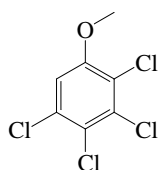
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 1600 mL g^{-1} d^{-1}$; $k_2 = 2.5 d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: biological $t_{1/2} < 1 d$ for all trichloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.9 2,3,4,5-Tetrachloroanisole

Common Name: 2,3,4,5-Tetrachloroanisole

Synonym:

Chemical Name:

CAS Registry No: 938-86-3

Molecular Formula: $C_7H_4Cl_4O$, $C_6HCl_4(OCH_3)$

Molecular Weight: 245.918

Melting Point ($^{\circ}C$):

88 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

210.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.241 (mp at $88^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.35 (shake flask-GC/ECD, Lun et al. 1995)

2.76 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzenes as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

1.202 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

153.0 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.51 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

4.50 (shake flask-GC/ECD, both phases, Lun et al. 1995)

4.57 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.78 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.67 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

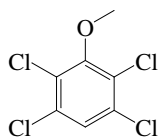
Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 940$ $mL\ g^{-1}\ d^{-1}$; $k_2 = 0.42\ d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: biological $t_{1/2} \sim 1-4$ d for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.10 2,3,5,6-Tetrachloroanisole



Common Name: 2,3,5,6-Tetrachloroanisole

Synonym:

Chemical Name:

CAS Registry No: 6936-40-9

Molecular Formula: $C_7H_4Cl_4O$, $C_6HCl_4(OCH_3)$

Molecular Weight: 245.918

Melting Point ($^{\circ}C$):

84 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

210.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.264 (mp at $84^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.82 (shake flask-GC/ECD, Lun et al. 1995)

3.64 (supercooled liquid S_L , RP-HPLC- k' correlation, using chlorobenzene as reference compound standard, Pfeifer et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$):

0.427 (supercooled liquid P_L , GC-RT correlation, Pfeifer et al. 2001)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

318.4 (calculated- P_L/C_L , Pfeifer et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.68 (RP-HPLC-capacity factor correlation, Opperhuizen & Voors 1987)

4.40 (shake flask-GC/ECD, both phases, Lun et al. 1995)

4.52 (RP-HPLC- k' correlation, Pfeifer et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.41 (calculated- K_{OW}/K_{AW} , Pfeifer et al. 2001)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.69 (guppy, concn ratio of C_{fish}/C_{water} , Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

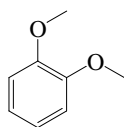
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 1480 mL g^{-1} d^{-1}$; $k_2 = 0.44 d^{-1}$ (guppy, continuous flow aqueous saturation system, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: biological $t_{1/2} \sim 1-4 d$ for all tetrachloro congeners (guppy, Opperhuizen & Voors 1987)

10.1.3.11 Veratrole (1,2-Dimethoxybenzene)

Common Name: Veratrole

Synonym: 1,2-dimethoxybenzene

Chemical Name: 1,2-dimethoxybenzene

CAS Registry No: 91-16-7

Molecular Formula: $C_8H_{10}O_2$, $C_6H_4(OCH_3)_2$

Molecular Weight: 138.164

Melting Point ($^{\circ}C$):

22 (Stephenson & Malanowski 1987)

22.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

206.7 (Stephenson & Malanowski 1987)

206 (Lide 2003)

Density (g/cm^3):

Molar Volume (cm^3/mol):

127.1 (calculated-density)

158.6 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

7160*, 7060 (19.9, $31^{\circ}C$, shake flask-GC, measured range 19.9 – $91.8^{\circ}C$, Stephenson 1992)

6690 (shake flask-HPLC/UV, Lun et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

$\log(P_L/kPa) = 8.705 - 3492/(T/K)$, temp range not specified (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.79 (Log P Database, Hansch & Leo 1987, quoted, Sangster 1993)

1.79 (HPLC-RT correlation, average value, Ritter et al. 1994)

1.60 (recommended, Hansch et al. 1995)

2.18 (shake flask-HPLC/UV both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

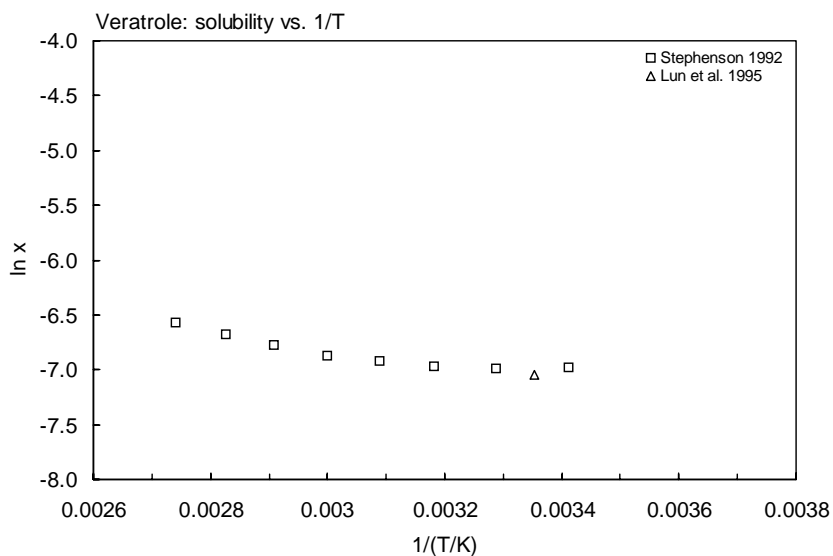
Sorption Partition Coefficient, $\log K_{OC}$:

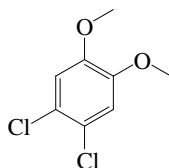
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.3.11.1**Reported aqueous solubilities of veratrole at various temperatures**

Stephenson 1992	
shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
19.9	7160
31	7060
41.1	7230
50.6	7580
60.2	7940
70.6	8770
80.7	9700
91.8	10730

**FIGURE 10.1.3.11.1** Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for veratrole.

10.1.3.12 4,5-Dichloroveratrole

Common Name: 4,5-dichloroveratrole

Synonym:

Chemical Name:

CAS Registry No: 2772-46-5

Molecular Formula: $C_8H_8Cl_2O_2$, $C_6H_2Cl_2(OCH_3)_2$

Molecular Weight: 207.054

Melting Point ($^{\circ}C$):

83 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

200.4 (Le-Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.27 (mp at $83^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

71.9 (shake flask-HPLC/UV, Lun et al. 1995)

72.6 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.11 (shake flask-GC/ECD, both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

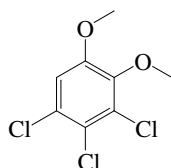
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.13 3,4,5-Trichloroveratrole



Common Name: 3,4,5-trichloroveratrole

Synonym:

Chemical Name:

CAS Registry No: 16766-29-3

Molecular Formula: $C_8H_7Cl_3O_2$, $C_6HCl_3(OCH_3)_2$

Molecular Weight: 241.499

Melting Point ($^{\circ}C$):

66 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

221.3 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.396 (mp at $66^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.50 (shake flask-GC, Neilson et al. 1984)

10.3 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.60, 5.25 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)

4.01 (shake flask-GC/ECD, both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

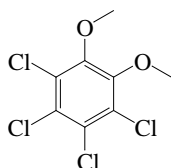
3.50, 3.30 (zebra fish, calculated, Neilson et al. 1984)

Sorption Partition Coefficient, $\log K_{oc}$:

3.20 (sediment, $K_p = 1.6 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.14 Tetrachloroveratrole

Common Name: Tetrachloroveratrole

Synonym: 1,2,3,4-tetrachloro-5,6-dimethoxybenzene

Chemical Name: tetrachloroveratrole

CAS Registry No: 944-61-6

Molecular Formula: $C_8H_6Cl_4O_2$, $C_6Cl_4(OCH_3)_2$

Molecular Weight: 275.944

Melting Point ($^{\circ}C$):

90 (Lun et al. 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.23 (mp at $90^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.70 (shake flask-GC, Neilson et al. 1984)

1.59 (shake flask-GC/ECD, Lun et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.80, 5.90 (HPLC-RT correlation, calculated-solubility, Neilson et al. 1984)

4.70 (Sarrikoski et al. 1986)

5.90 (Part et al. 1992, quoted, Sangster 1993)

4.86 (shake flask-GC/ECD both phases, Lun et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.40, 4.50 (zebra fish, calculated, Neilson et al. 1984)

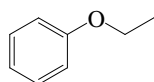
Sorption Partition Coefficient, $\log K_{oc}$:

3.45 (sediment, $K_p = 2.8 ml \cdot (kg \text{ of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.3.15 Phenetole



Common Name: Phenetole

Synonym: ethoxybenzene, ethyl phenyl ether

Chemical Name: ethoxybenzene, ethyl phenyl ether

CAS Registry No: 103-73-1

Molecular Formula: $C_8H_{10}O$, $C_6H_5-O-C_2H_5$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

-29.52 (Riddick et al. 1986)

-33.00 (Stephenson & Malanowski 1987)

-29.43 (Lide 2003)

Boiling Point ($^{\circ}C$):

169.84 (Riddick et al. 1986)

172.00 (Stephenson & Malanowski 1987)

169.81 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9651, 0.9605 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949; Riddick et al. 1986)

Molar Volume (cm^3/mol):

126.6 ($20^{\circ}C$, calculated-density)

150.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1160 (residual volume, Booth & Everson 1948)

550 (shake flask-AS, McGowan et al. 1966)

569 (shake flask-UV, Vesala 1974)

1114 (calculated- K_{ow} , Valvani et al. 1981)

1200 (selected, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($18^{\circ}C$, compiled and evaluated data, temp range $18-172^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.40281 - 1808.8/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

7605* ($91.89^{\circ}C$, ebulliometry, measured range $91.89-170^{\circ}C$, Dreisbach & Shrader 1949)

20441* ($117.43^{\circ}C$, ebulliometry, measured range $117.43-180.608^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.01980 - 1507.267/(194.357 + t/^{\circ}C)$; temp range $117.43-180.608^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 24.97404 - 3295.20/(T/K) - 5.53743 \cdot \log(T/K)$; temp range $117.43-180.608^{\circ}C$ (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)

204* (comparative ebulliometry-extrapolated, measured range $117.438-180.642^{\circ}C$, Ambrose et al. 1976)

$\log(P/kPa) = 6.14658 - 1509.276/\{(T/K) - 78.502\}$; temp range $391-454 K$ (Antoine eq., Ambrose et al. 1976)

$\log(P/kPa) = 6.17151 - 1529.38/(197.132 + t/^{\circ}C)$; temp range $91.89-170^{\circ}C$ (Antoine eq. derived from exptl data of Dreisbach & Martin 1949, Boublik et al. 1984)

$\log(P/kPa) = 6.14656 - 1508.583/(194.512 + t/^{\circ}C)$; temp range $117.4-180.68^{\circ}C$ (Antoine eq. derived reported exptl data of Collerson et al. 1965, Boublik et al. 1984)

204 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.14658 - 1509.276/(194.648 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.14524 - 1508.326/(-78.613 + T/\text{K})$; temp range 390–454 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -8.3543 - 2.7728 \times 10^3/(T/\text{K}) + 9.4482 \cdot \log (T/\text{K}) - 2.1842 \times 10^{-2} \cdot (T/\text{K}) + 1.1038 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 244–647 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

44.5 (calculated-P/C from selected data)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

2.51 (shake flask, Hansch & Leo 1979; 1987)

2.68 (HPLC- k' correlation, Haky & Young 1984)

2.51 (recommended, Sangster 1993)

2.51 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.3.15.1

Reported vapor pressures of phenetole at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
18.1	133.3	91.89	7605	117.432	20441	117.438	20441
43.7	666.6	95.6	8850	124.908	26526	124.918	26526
56.4	1333	98.84	10114	131.478	33024	131.49	33024
70.3	2666	111.56	16500	137.43	39978	137.445	39978
86.6	5333	139.17	42066	142.338	46566	142.355	46566
95.4	7999	155.16	67661	146.908	53454	146.927	53453
108.4	13332	170	101325	150.795	59940	150.816	59940
127.9	26664			154.432	66655	154.455	66570
149.8	53329			157.829	73278	157.853	73277
172	101325	Antoine eq. given by		160.982	79972	161.008	79972
		Dreisbach & Martin 1949		163.972	86762	163.999	86762
mp/°C	–30.2	eq. 2	P/mmHg	166.622	93152	166.65	93152
		A	7.40281	169.315	100033	169.344	100033
		B	1808.8	171.821	106789	171.852	106788
		C	230	174.19	113487	174.221	113486
				176.407	120058	176.439	120057
		bp/°C	170	178.511	126572	178.544	126571
		mp/°C	–29.52	180.608	133334	180.642	133334
						25	204

(Continued)

TABLE 10.1.3.15.1 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1976	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				bp/°C	169.806		
				Antoine eq.		Antoine eq.	
				eq. 2	P/mmHg	eq. 2	P/kPa
				A	7.0198	A	6.14658
				B	1507.267	B	1509.276
				C	194.357	C	−78.502
				Kirchhoff eq.		Coefficients of Chebyshev eq. also given in text.	
				eq. 4	P/mmHg		
				A	24.97404		
				B	3295.2		
				C	5.53743		
				ΔH _v /(kJ mol ^{−1}) = 40.71			

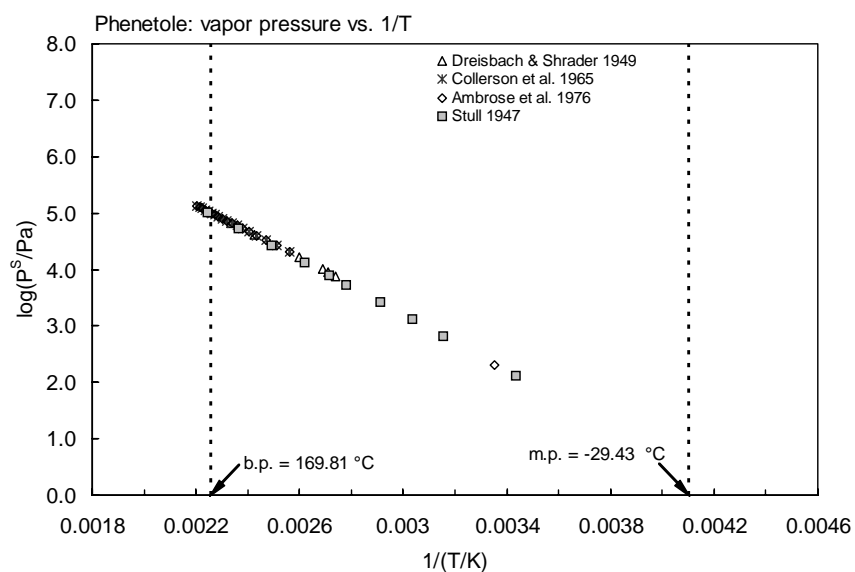
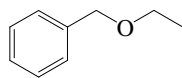


FIGURE 10.1.3.15.1 Logarithm of vapor pressure versus reciprocal temperature for phenetole.

10.1.3.16 Benzyl ethyl ether



Common Name: Benzyl ethyl ether

Synonym: (ethoxymethyl)benzene, α -ethoxytoluene

Chemical Name: benzyl ethyl ether, (ethoxymethyl)benzene, α -ethoxytoluene

CAS Registry No: 539-30-0

Molecular Formula: $C_9H_{12}O$, $C_6H_5CH_2-O-C_2H_5$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

185.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9490 (Weast 1982–83)

0.9478 (Dean 1985)

Molar Volume (cm^3/mol):

143.5 ($20^{\circ}C$, calculated-density)

172.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

135* (calculated-Antoine eq. regression, Stull 1947)

100 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.6496 - 1927.21/(230 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

135 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.92406 - 2133.29/(-24.38 + T/K)$; temp range 299–460 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 27.6421 - 3.4249 \times 10^3/(T/K) - 6.5804 \cdot \log(T/K) + 9.3417 \times 10^{-10} \cdot (T/K) + 1.0547 \times 10^{-6} \cdot (T/K)^2$; temp range 309–660 K (vapor pressure eq., Yaws 1994)

95.44* ($25.35^{\circ}C$, transpiration method, measured range 278.3–313.7 K, Krasnykh et al. 2002)

$\ln(P/Pa) = (305.859/R) - [79968.084/R(T/K)] - (88.80/R) \cdot \ln[(T/K)/298.15]$; temp range 278–313.7 K (transpiration method, Krasnykh et al. 2002)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.64 (calculated-f const. as per Rekker 1977, Hanai et al. 1981)

2.16 (Wang et al. 1987)

2.16 (recommended, Sangster 1993)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (Darnall et al. 1976).

TABLE 10.1.3.16.1

Reported vapor pressures of benzyl ethyl ether at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Krasnykh et al. 2002			
summary of lit. data		transpiration method			
t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
26	133	278.3	19.44	298.6	95.44
52	666.6	278.7	19.59	300.1	105.16
65	1333	283.8	30.11	302.3	117.65
79.6	2666	285.1	35.31	303.2	128.09
95.4	5333	288.8	44.78	303.6	135.21
105.5	7999	290.2	52.97	307.4	177.63
118.9	13332	292.6	61.54	308.4	188.48
139.6	26664	293.7	65.53	310.2	223.55
161.5	53329	295.2	77.81	312.2	244.83
185	101325	297.3	88.33	313.7	259.37

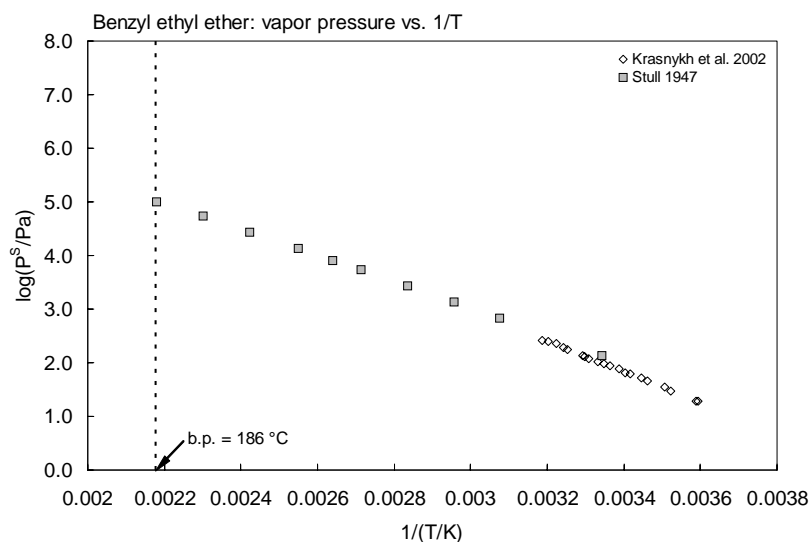
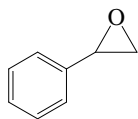


FIGURE 10.1.3.16.1 Logarithm of vapor pressure versus reciprocal temperature for benzyl ethyl ether.

10.1.3.17 Styrene oxide



Common Name: Styrene oxide

Synonym: (1,2-epoxyethyl)benzene, phenylepoxyethane

Chemical Name: (1,2-epoxyethyl)benzene, phenylepoxyethane, styrene oxide

CAS Registry No: 96-09-3

Molecular Formula: C_8H_8O

Molecular Weight: 120.149

Melting Point ($^{\circ}C$):

-35.6 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

194.1 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0523 ($16^{\circ}C$, Weast 1982–83; Dean 1985)

1.0500 (Verschueren 1983)

Molar Volume (cm^3/mol):

114.4 ($20^{\circ}C$, calculated-density)

136.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2800 (quoted, Verschueren 1983)

3020; 4570 (quoted exptl.; calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

40.0 (Verschueren 1983)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.84 (shake flask-HPLC, Pratesi et al. 1979)

1.51 (shake flask-GC, Serrentino et al. 1983)

1.61 (shake flask, Log P Database, Hansch & Leo 1987)

1.43 (Deneer et al. 1988)

1.61 (recommended, Sangster 1989, 1993)

1.51 (pH 7.5, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} = 12.3\text{--}123$ h, based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: rate constants $k = (434 \pm 12) \times 10^{-8} s^{-1}$ at pH 7.25 and $k = (1690 \pm 620) \times 10^{-8} s^{-1}$ at pH 7.3 in sediment pores both at $25^{\circ}C$ for water containing 0.1% w/w CH_2O as sterilant with 1-phenyl-1,2-ethanediol as major hydrolyzed product (Haag & Mill 1988);

$t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C, the hydrolysis half-lives at pH 5, 7 and 9 are 0.00385, 21.4 and 27.5 h (Haag & Mill 1988; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on biological screening test data (Schmidt-Bleek et al. 1982; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24$ h from air for the reaction with OH radical (US EPA 1974; quoted, Darnall et al. 1976);

$t_{1/2} = 12.3\text{--}123$ h, based on estimated photooxidation rate constant with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: $t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

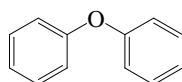
Ground water: $t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 0.00385\text{--}27.5$ h, based on an estimation from measured first-order rate constants at 25°C (Haag & Mill 1988; quoted, Howard et al. 1991).

Biota:

10.1.3.18 Diphenyl ether



Common Name: Diphenyl ether

Synonym: phenyl ether, diphenyl oxide, phenyl ether, 1,1'-oxybisbenzene, phenoxybenzene

Chemical Name: diphenyl ether, diphenyloxide, phenylether, phenoxybenzene

CAS Registry No: 101-84-8

Molecular Formula: $C_{12}H_{10}O$, $(C_6H_5)_2O$

Molecular Weight: 170.206

Melting Point ($^{\circ}C$):

26.87 (Lide 2003)

Boiling Point ($^{\circ}C$):

258 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0748 (Weast 1982–83)

Molar Volume (cm^3/mol):

158.6 ($20^{\circ}C$, calculated-density)

166.6 (Ruelle & Kesselring 1997)

195.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.217 (quoted, Riddick et al. 1986)

16.16 (Ruelle & Kesselring 1997)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 0.923 (mp $28.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4000 (shake flask-residue-volume, Booth & Everson 1948)

18.7 (shake flask-UV, Vesala 1974)

18.0 (shake flask-HPLC, Banerjee et al. 1980; Pearlman et al. 1984)

21.0 (Verschuereen 1983)

18, 3900 (quoted values, Riddick et al. 1986)

46.88 (supercooled liquid S_L , RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($66.1^{\circ}C$, summary of literature data, temp range 66.1 – $258.5^{\circ}C$, Stull 1947)

10.01* ($40^{\circ}C$, dynamic method, measured range 40 – $60^{\circ}C$, Bent & Francel 1948)

$\log(P/mmHg) = 9.6842 - 3351.9/(t/^{\circ}C + 273.1)$; measured range 40 – $60^{\circ}C$ (dynamic method-gas saturation, Bent & Francel 1948)

$\log(P/mmHg) = 7.65339 - 2330.5/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

26555* ($204.213^{\circ}C$, ebulliometry, measured range 204.2 – $270.9^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.06376 - 1261.455/(221.982 + t/^{\circ}C)$; temp range 204.2 – $270.9^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 19.48322 - 2328.0/(T/K) - 3.92657 \cdot \log(T/K)$; temp range 204.2 – $270.9^{\circ}C$ (Krichhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = [-0.2185 \times 12325.5/(T/K)] + 7.955679$; temp range 66.1 – $258.5^{\circ}C$ (Antoine eq., Weast 1972–73)

3.0* (“recomputed” reported data, temp range 204.257 – $271^{\circ}C$, Ambrose et al. 1976)

$\log(P/kPa) = 6.13913 - 1802.984/\{(T/K) - 95.013\}$; temp range 477 – $544\ K$ (Antoine eq., Ambrose et al. 1976)

2.67 (Verschuereen 1983)

1.82 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.01104 - 1799.712/(177.744 + t/^{\circ}C)$; temp range 204 – $270^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.13606 - 1799.811/(177.756 + t/^{\circ}\text{C})$; temp range 204.2–271 $^{\circ}\text{C}$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log (P/\text{mmHg}) = 7.01104 - 1799.71/(177.74 + t/^{\circ}\text{C})$; temp range: 204–271 $^{\circ}\text{C}$ (Antoine eq., Dean 1985, 1992)
2.84 (selected, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.13913 - 1902.984/(178.137 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
2.93 (calculated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{kPa}) = 8.7109 - 3351.9/(T/\text{K})$; temp range 313–333K (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log (P/\text{kPa}) = 6.1553 - 1800.743/(T/\text{K} - 95.275)$; temp range 477–544K (Antoine eq., liquid, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -26.9635 - 2.5909 \times 10^3/(T/\text{K}) + 16.42 \cdot \log (T/\text{K}) - 2.4334 \times 10^{-2} \cdot (T/\text{K}) + 1.0244 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 300–763 K (vapor pressure eq., Yaws 1994)

2.40 (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25 $^{\circ}\text{C}$):

25.1 (calculated-P/C using selected data)

8.71 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.21, 4.36 (shake flask values, Leo et al. 1971)

4.20 (shake flask-GC, Chiou et al. 1977)

4.25 (calculated-fragment const., Rekker 1977)

4.26 (Hansch & Leo 1979)

4.08 (shake flask-HPLC, Banerjee et al. 1980)

3.79 (estimated-HPLC/MS correlation, Burkhard et al. 1985)

4.24 (calculated-f const., Burkhard et al. 1985)

3.87 (HPLC-RT correlation, Eadsforth 1986)

4.28 (shake flask, Log P Database, Hansch & Leo 1987)

4.21 (recommended, Sangster 1989, 1993)

3.949, 4.014 (shake flask method, Brooke et al. 1990)

4.21 (recommended, Hansch et al. 1995)

3.97 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.42 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log \text{BCF}$:

2.29 (rainbow trout, calculated, Veith et al. 1979)

2.29; 2.89 (quoted exptl., calculated- K_{OW} , Mackay 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

3.29; 3.41 (soil, quoted exptl.; calculated-MCI χ , Meylan et al. 1992)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_1 = 5.5 \text{ h}^{-1}$, $k_2 = 0.0275 \text{ h}^{-1}$ (trout, Hawker & Connell 1985)

$1/k_2 = 36 \text{ h}$ (trout, Hawker & Connell 1988)

$k_2 = 0.676 \text{ h}^{-1}$ (fish, quoted, Thomann 1989)

Half-Lives in the Environment:

Air: disappearance $t_{1/2} < 0.24 \text{ h}$ from air for the reaction with OH radical (USEPA 1974; quoted, Darnall et al. 1976).

TABLE 10.1.3.18.1

Reported vapor pressures of diphenyl ether at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Bent & Francel 1948		Collerson et al. 1965		Ambrose et al. 1976	
summary of lit. data		dynamic method		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
66.1	133.3	40	10.01	204.13	26555	204.257	26555
97.8	666.6	50	21.96	212.102	33073	212.15	33074
114	1333	60	43.97	219.226	40022	219.276	40022
130.8	2666			225.105	46611	225.157	46611
150	5333	eq. 2	P/mmHg	230.561	53482	230.616	53481
162	7999	A	9.5842	235.186	59915	235.242	59915
178.8	13332	B	3351.9	239.618	66654	239.676	66654
203	26664	C	273.1	243.667	73327	243.726	73327
230.7	53329			250.991	86741	247.473	79956
258.5	101325	ΔH _v = 64.02 kJ/mol		254.089	92971	251.052	86740
				257.458	100143	254.152	92971
mp/°C	27			260.469	106906	257.522	100144
				263.29	113569	260.534	106906
				268.939	120124	263.355	113568
		Dreisbach & Shrader 1949		268.416	126525	266.005	120124
		ebulliometry		270.949	133333	268.482	126525
		No data				271.015	133332
				bp/°C	257.997	25	3
		Antoine eq. given by		Antoine eq.			
		Dreisbach & Martin 1949		eq. 2	P/mmHg	bp	531.21 K
		eq. 2	P/mmHg	A	7.01188	Antoine equation:	
		A	7.65339	B	1800.415	eq. 3	P/kPa
		B	2330.5	C	177.826	A	6.12913
		C	230	Kirchhoff eq.		B	1802.984
				eq. 4	P/mmHg	C	–95.013
		bp/°C	258.31	A	24.66548	Coefficients of Chebyshev eq. also given in text.	
		mp/°C	26.9	B	3897.5		
				C	5.30117		
ΔH _v = 48.62 kJ/mol							

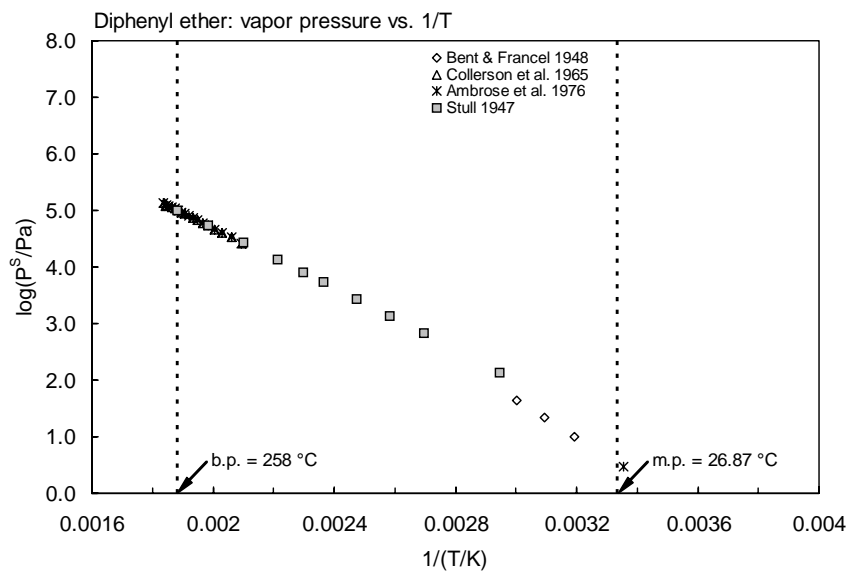
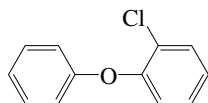


FIGURE 10.1.3.18.1 Logarithm of vapor pressure versus reciprocal temperature for diphenyl ether.

10.1.4 POLYCHLORINATED DIPHENYL ETHERS (PCDEs)

10.1.4.1 2-Chlorodiphenyl ether (PCDE-1)



Common Name: 2-Chlorodiphenyl ether

Synonym: 2-CDPE, PCDE-1, 2-chlorobiphenyl ether

Chemical Name: 2-chlorodiphenyl ether

CAS Registry No: 2689-07-8

Molecular Formula: $C_{12}H_9ClO$

Molecular Weight: 204.652

Melting Point ($^{\circ}C$):

45 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

216.5 (calculated-Le Bas method at normal boiling point)

179.5 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.634 (mp at $45^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.40; 4.80 (quoted exptl.; calculated-molar volume and MP, Ruelle & Kesselring 1997)

3.40 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.537 (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

32.36 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.45 (HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.33 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Photolysis: photolysis rate $k_p = 0.0035$ d^{-1} with a half-life of 200 d in summer sunlight; $k_p(exptl) = 3.4 \times 10^{-8}$ s^{-1} with $t_{1/2} = 240$ h, $k_p(calc) = 3.1 \times 10^{-9}$ s^{-1} in winter sunlight, at $40^{\circ}C$ in surface waters (Dulin et al. 1986)

Half-Lives in the Environment:

Air:

Surface water: photolysis $t_{1/2} = 200$ d in summer sunlight and $t_{1/2} = 240$ d in winter sunlight at $40^{\circ}C$ in surface waters (Dulin et al. 1986)

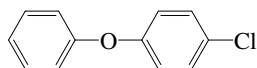
Ground water:

Sediment:

Soil:

Biota: $t_{1/2} = 4-63$ d in trout Cl_1 -DPEs to Cl_4 -DPEs (Niimi et al. 1994).

10.1.4.2 4-Chlorodiphenyl ether



Common Name: 4-Chlorodiphenyl ether

Synonym: 4-chlorophenyl phenyl ether, 1-chloro-4-phenoxybenzene, p-chlorophenyl phenyl ether, 4-chlorodiphenyl ether, monochlorodiphenyl oxide

Chemical Name: 4-chlorophenyl phenyl ether, 4-chlorodiphenyl ether

CAS Registry No: 7005-72-3

Molecular Formula: $C_{12}H_9ClO$

Molecular Weight: 204.652

Melting Point ($^{\circ}C$):

−6.0 (Callahan et al. 1979)

−8.0 (Mabey et al. 1982)

Boiling Point ($^{\circ}C$):

284.5 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2026 ($15^{\circ}C$, Weast 1982–83; Lide 2003)

Molar Volume (cm^3/mol):

216.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.30 (Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

59.04 (Isnard & Lambert 1988,1989)

Vapor Pressure (Pa at $25^{\circ}C$):

0.360 (calculated, Branson 1977; quoted, Callahan et al. 1979; Mabey et al. 1982)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$ or as indicated):

22.19 (calculated-P/C, Mabey et al. 1982)

22.29 (20 – $25^{\circ}C$ and low ionic strength, quoted, Pankow & Rosen 1988; Pankow 1990)

24.79 (quoted from WERL Treatability Data, Ryan et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.08 (Branson 1977; quoted, Callahan et al. 1979; Ryan et al. 1988; Isnard & Lambert 1988,1989)

5.079 (calculated, Mabey et al. 1982)

Bioconcentration Factor, $\log BCF$:

2.867 (rainbow trout muscle, Branson 1977; quoted, Callahan et al. 1979)

4.255 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)

2.87 (quoted, Isnard & Lambert 1988)

Sorption Partition Coefficient, $\log K_{oc}$:

4.763 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photolysis rate $k_p = 0.19 d^{-1}$ with $t_{1/2} = 3.6 d$ in summer sunlight; $k_p(exptl) < 2.0 \times 10^{-8} s^{-1}$ with $t_{1/2} > 400 h$, $k_p(calc) = 3.7 \times 10^{-8} s^{-1}$ in winter sunlight, both at $40^{\circ}C$ in surface waters (Dulin et al. 1986)

Oxidation: $k \ll 360 M^{-1} h^{-1}$ for singlet oxygen and $k \ll 1.0 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982)

Hydrolysis:

Biodegradation: $t_{1/2} = 4.0$ h, measured only in activated sludge (Branson 1978; quoted, Callahan et al. 1979).

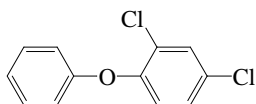
Biotransformation: estimated rate constant $k = 1 \times 10^{-7}$ mL cell⁻¹ h⁻¹ for bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

Surface water: photolysis $t_{1/2} = 3.6$ d summer sunlight and $t_{1/2} > 400$ d in winter sunlight at 40° L surface waters (Dulin et al. 1986)

10.1.4.3 2,4-Dichlorodiphenyl ether (PCDE-8)



Common Name: 2,4-Dichlorodiphenyl ether

Synonym: 2,4-DCDPE, PCDE-8

Chemical Name:

CAS Registry No: 51892-26-3

Molecular Formula: $C_{12}H_8Cl_2O$

Molecular Weight: 239.097

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

237.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.605 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.123 (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.25 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.62 (Oliver & Niimi 1984)

4.93 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.60 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

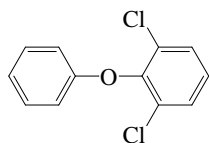
3.97 (rainbow trout, Oliver & Niimi 1984)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 3-63\ d$ for Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.4 2,6-Dichlorodiphenyl ether (PCDE-10)

Common Name: 2,6-Dichlorodiphenyl ether

Synonym: 2,6-DCDPE, PCDE-10

Chemical Name:

CAS Registry No: 28419-69-4

Molecular Formula: $C_{12}H_8Cl_2O$

Molecular Weight: 239.097

Melting Point ($^{\circ}C$):

39 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

237.4 (calculated-Le Bas method at normal boiling point)

192.4 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.729 (mp at $39^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.08; 0.213 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

2.08 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.174 (supercooled liquid P_L , GC-RI correlation, Kurz & Kesselring 1997)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

19.95 (calculated-P/C, Kurz & Kesselring 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.64 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.73 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

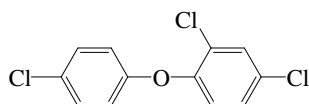
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 4-63$ d Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.5 2,4,4'-Trichlorodiphenyl ether (PCDE-28)



Common Name: 2,4,4'-Trichlorodiphenyl ether

Synonym: 2,4,4'-TCDPE, PCDE-28

Chemical Name: 2,4,4'-trichlorodiphenyl ether

CAS Registry No: 59030-21-3

Molecular Formula: $C_{12}H_7Cl_3O$

Molecular Weight: 273.543

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

40 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

258.3 (calculated-Le Bas method at normal boiling point)

205.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.712 (mp at $40^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.102; 0.0385 (quoted exptl.; calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.101 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0204 (supercooled liquid P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

33.88 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.53 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.19 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.98; 3.36 (concn of 2,4,4'-trichloro-DPE 39.3; 118 $\mu g/L$, juvenile Atlantic salmon, 96-h exposure, Zitko & Carson 1977)

Sorption Partition Coefficient, $\log K_{OC}$:

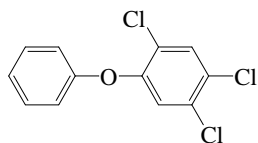
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 235$ h following uptake from water, excretion $t_{1/2} = 15$ d following uptake from food for Juvenile salmon (Zitko & Carson 1977);

average $t_{1/2} = 15$ d in salmon for trichloro-DPE congeners; biological $t_{1/2} = 63$ d (range 46–104 d) in rainbow trout (average value for trichlorodiphenyl ethers (Niimi 1986);

$t_{1/2} = 4$ –63 d Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.6 2,4,5-Trichlorodiphenyl ether (PCDE-29)

Common Name: 2,4,5-Trichlorodiphenyl ether

Synonym: 2,4,5-TCDPE, PCDE-29

Chemical Name: 2,4,5-trichlorodiphenyl ether

CAS Registry No: 52322-80-2

Molecular Formula: $C_{12}H_7Cl_3O$

Molecular Weight: 273.543

Melting Point ($^{\circ}C$):

oil (Opperhuizen & Voors 1987)

61 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

258.3 (calculated-Le Bas method at normal boiling point)

205.3 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.443 (mp at $61^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.050 (Opperhuizen 1986)

0.072; 0.0486 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.072 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0288 (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

112.2 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.0 (estimated, Opperhuizen 1986)

5.44 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)

5.58 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

6.92 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.18 (guppy, 8-d exposure, Opperhuizen & Voors 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Biotransformation: rate of metabolism $k = 0.27$ d^{-1} (guppy, 8-d exposure, Opperhuizen & Voors 1987)

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

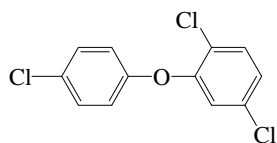
$k_1 > 5 \times 10^2$ d^{-1} (guppy, Opperhuizen 1986)

$k_1 = 1.5 \times 10^3$ mL g^{-1} d^{-1} (guppy, 8-d exposure, Opperhuizen & Voors 1987)

$k_2 = 0.34$ d^{-1} (guppy, elimination period 56 d, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: average excretion $t_{1/2} = 15$ d for trichloro-DPE congeners in salmon; biological $t_{1/2} = 63$ d in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);
 $t_{1/2} = 4\text{--}63$ d for Cl₁-DPEs to Cl₄-DPEs in trout (Niimi et al. 1994).

10.1.4.7 2,4',5-Trichlorodiphenyl ether (PCDE-31)

Common Name: 2,4',5-Trichlorodiphenyl ether

Synonym: 2,4',5-TCDPE, PCDE-31

Chemical Name: 2,4',5-trichlorodiphenyl ether

CAS Registry No: 65075-00-5

Molecular Formula: $C_{12}H_7Cl_3O$

Molecular Weight: 273.543

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

258.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0993 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0229 (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.31 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.66 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

5.70 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.25 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.30; 2.93 (ave. concn of 2,4',5-trichloro-DPE 2.37; 7.01 $\mu g/L$, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, $\log K_{OC}$:

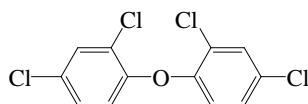
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 310\ h$ following uptake from water; $t_{1/2} = 26\ d$ following uptake from food for juvenile Atlantic salmon (Zitko & Carson 1976);

average excretion $t_{1/2} = 15\ d$ for trichloro-DPE congeners in salmon; biological $t_{1/2} = 63\ d$ in rainbow trout (average value for trichlorodiphenyl ethers, Niimi 1986);

$t_{1/2} = 4\text{--}63\ d$ Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.8 2,2',4,4'-Tetrachlorodiphenyl ether (PCDE-47)

Common Name: 2,2',4,4'-Tetrachlorodiphenyl ether

Synonym: 2,2',4,4'-TCDPE, PCDE-47, 2,2',4,4'-tetrachlorobiphenyl ether, 2,2',4,4'-TCBP

Chemical Name: 2,2',4,4'-tetrachlorodiphenyl ether

CAS Registry No: 28076-73-5

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

69–70 (Navalainen et al. 1994)

69 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

218.2 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.366$ (mp at $69.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0466; 0.0154 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.0466 (supercooled liquid, RP-HPLC-RI, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00525 (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

34.67 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.95 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{AO}$:

7.80 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

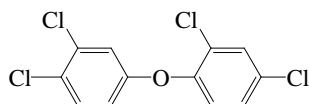
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: average excretion $t_{1/2} = 55\ d$ in salmon for tetrachloro-DPE congeners; mean biological $t_{1/2} = 119\ d$ (range 82–213 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 4$ –63 d for Cl_1 -DPEs to Cl_4 -DPEs in trout (Niimi et al. 1994).

10.1.4.9 2,3',4,4'-Tetrachlorodiphenyl ether (PCDE-66)

Common Name: 2,3',4,4'-Tetrachlorodiphenyl ether

Synonym: 2,3',4,4'-DCPE, PCDE-66

Chemical Name: 2,3',4,4'-tetrachlorodiphenyl ether

CAS Registry No: 61328-46-9

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0308 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

0.00407 (supercooled liquid P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

40.74 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.13 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{AO}$:

7.91 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.43; 3.01 (ave. concn of 2,3',4,4'-tetrachloro-DPE 2.07; 6.03 $\mu g/L$, juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

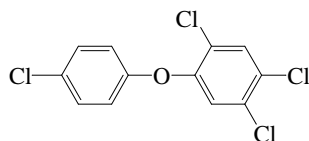
Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 370$ h following uptake from water, $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);

average excretion $t_{1/2} = 55$ d in salmon for tetrachloro-DPE congeners; mean biological $t_{1/2} = 119$ d (range 82–213 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 4$ –63 d in trout for Cl_1 -DPEs to Cl_4 -DPEs (Niimi et al. 1994).

10.1.4.10 2,4,4',5-Tetrachlorodiphenyl ether (PCDE-74)



Common Name: 2,4,4',5-Tetrachlorodiphenyl ether

Synonym: 2,4,4',5-PCDE, PCDE-74

Chemical Name: 2,4,4',5-tetrachlorodiphenyl ether

CAS Registry No: 61328-45-8

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

62–63 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0281 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

4.79×10^{-3} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

52.48 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.99 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.66 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

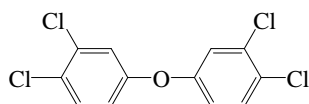
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986); mean biological $t_{1/2} = 108$ d (range 62–407 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 4$ –63 d in trout for Cl_1 -DPEs to Cl_4 -DPEs; $t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.11 3,3',4,4'-Tetrachlorodiphenyl ether (PCDE-77)

Common Name: 3,3',4,4'-Tetrachlorodiphenyl ether

Synonym: 3,3',4,4'-PCDE, PCDE-77

Chemical Name: 3,3',4,4'-tetrachlorodiphenyl ether

CAS Registry No: 56348-72-2

Molecular Formula: $C_{12}H_6Cl_4O$

Molecular Weight: 307.988

Melting Point ($^{\circ}C$):

oil (Opperhuizen & Voors 1987)

69–71 (Navalainien et al. 1994)

70 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

279.2 (calculated-Le Bas method at normal boiling point)

218.2 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.362 (mp at $70^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.020 (Opperhuizen 1986)

0.0323; 0.00991 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.0323 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

2.57×10^{-3} (P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

24.55 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.0 (estimated, Opperhuizen 1986)

5.78 (Opperhuizen & Voors 1987; quoted, Niimi et al. 1994)

6.36 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.36 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

4.50 (guppy, 8-d exposure, Opperhuizen & Voors 1987)

4.51; 4.09 (guppy; trout muscle, Niimi et al. 1994)

4.46–4.99 (calculated- K_{OW} , Niimi et al. 1994)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 > 5 \times 10^2$ d⁻¹ (Guppy, Opperhuizen 1986)

$k_1 = 9.6 \times 10^2 \text{ mL g}^{-1} \text{ d}^{-1}$ (guppy, 8-d exposure, Opperhuizen & Voors 1987)

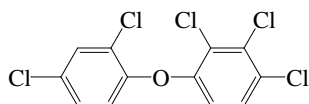
$k_2 = 0.03 \text{ d}^{-1}$ (guppy, elimination period 56 d, Opperhuizen & Voors 1987)

Half-Lives in the Environment:

Biota: average $t_{1/2} = 55 \text{ d}$ in salmon for tetrachloro-DPE congeners (Zitko & Carson 1977; quoted, Niimi 1986)

mean biological $t_{1/2} = 134 \text{ d}$ (range 73–792 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 23 \text{ d}$ in guppy, $t_{1/2} = 29 \text{ d}$ in trout muscle (Niimi et al. 1994).

10.1.4.12 2,2',3,4,4'-Pentachlorodiphenyl ether (PCDE-85)

Common Name: 2,2',3,4,4'-Pentachlorodiphenyl ether

Synonym: PDCE-85

Chemical Name: 2,2',3,4,4'-pentachlorodiphenyl ether

CAS Registry No: 71585-37-0

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

65–67 (Navalainen et al. 1994)

66 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.396 (mp at $66^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.0124; 0.00609 (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.0124 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

6.92×10^{-4} (supercooled liquid P_L , GC-RI correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

19.05 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.28 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.39 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

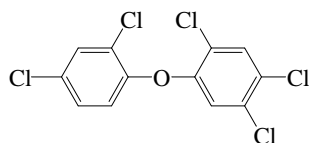
Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986)

biological $t_{1/2} \sim 113$ d (range 81–144 d, average value for pentachloro-DPE congeners, Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.13 2,2',4,4',5-Pentachlorodiphenyl ether (PCDE-99)



Common Name: 2,2',4,4',5-Pentachlorodiphenyl ether

Synonym: 2,2',4,4',5-PCDE, PCDE-99

Chemical Name: 2,2',4,4',5-pentachlorodiphenyl ether

CAS Registry No: 60123-64-0

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

25 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.5 (calculated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

1.0 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

5.06×10^{-3} ; 0.0153 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

8.406×10^{-3} (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.392 - 866.2/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.35×10^{-3} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

1.34×10^{-3} ; 1.34×10^{-3} (liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 11.90 - 4404/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.95 - 3525/(T/K)$ (liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

54.95 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa m^3/mol)] = 10.34 - 2659/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.38 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.46, 7.20 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.03 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

3.15; 2.77 (4.01; 12.0 $\mu g/L$, ave. concn of 2,2',4,4',5-PCDPE (reported as 2,2'4',5-TCDDPE), juvenile Atlantic salmon, 96-d exposure, Zitko & Carson 1976)

Sorption Partition Coefficient, $\log K_{OC}$:

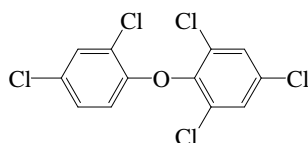
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 370$ h following uptake from water, $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);

average excretion $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners; mean biological $t_{1/2} = 144$ d (range 93–311 d) in rainbow trout (Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.14 2,2',4,4',6-Pentachlorodiphenyl ether (PCDE-100)

Common Name: 2,2',4,4',6-Pentachlorodiphenyl ether

Synonym: 2,2',4,4',6-PCDE, PCDE-100

Chemical Name: 2,2',4,4',6-pentachlorodiphenyl ether

CAS Registry No: 104294-16-8

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

45–46 (Navalainen et al. 1994)

46 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (calculated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

1.0 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

0.0160 (supercooled liquid value, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.392 - 943.0/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.19×10^{-3} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

2.17×10^{-3} ; 1.34×10^{-3} (liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 11.90 - 4408/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 8.95 - 3467/(T/K)$ (liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

46.77 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 10.34 - 2524/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.11 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.11, 6.31 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.83 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B :

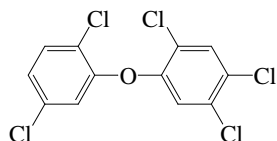
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

- Biota: excretion $t_{1/2} = 370$ h following uptake from water, $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1977);
- average excretion $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners; mean biological $t_{1/2} = 144$ d (range 93–311 d) in rainbow trout (Niimi 1986);
- $t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.15 2,2',4,5,5'-Pentachlorodiphenyl ether (PCDE-101)



Common Name: 2,2',4,5,5'-Pentachlorodiphenyl ether

Synonym: PDCE-101

Chemical Name: 2,2',4,5,5'-pentachlorodiphenyl ether

CAS Registry No: 131138-21-1

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

oil (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00943; 0.0153 (quoted exptl.; calculated-molar volume and mp, Ruelle & Kesselring 1997)

0.00943 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

1.74×10^{-3} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

63.10 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.22 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.81 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

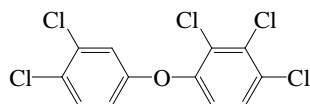
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: excretion $t_{1/2} = 370$ d following uptake from water; $t_{1/2} = 55$ d following uptake from food in juvenile Atlantic salmon (Zitko & Carson 1976);
average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977; Niimi 1986);
biological $t_{1/2} = 113$ d (range 81–144 d) in rainbow trout (average value of pentachloro-DPE, Niimi 1986);
 $t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.16 2,3,3',4,4'-Pentachlorodiphenyl ether (PCDE-105)

Common Name: 2,3,3',4,4'-Pentachlorodiphenyl ether

Synonym: PCDE-105

Chemical Name: 2,3,3',4,4'-pentachlorodiphenyl ether

CAS Registry No: 85918-31-6

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 324.433

Melting Point ($^{\circ}C$):

64–66 (Navalainen et al. 1994)

65 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

231.1 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.405 (mp at $65^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00732; 0.0059 (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

0.00732 (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

5.13×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

23.99 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.51 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.52 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

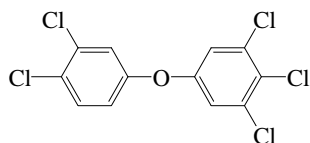
Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)

biological $t_{1/2} \sim 113$ d (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.17 3,3',4,4',5-Pentachlorodiphenyl ether (PCDE-126)



Common Name: 3,3',4,4',5-Pentachlorodiphenyl ether

Synonym: PCDE-126

Chemical Name: 3,3',4,4',5-pentachlorodiphenyl ether

CAS Registry No: 94339-59-0

Molecular Formula: $C_{12}H_5Cl_5O$

Molecular Weight: 342.433

Melting Point ($^{\circ}C$):

68–70 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

300.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.93×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

5.62×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

100 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.83 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.88 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.22 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

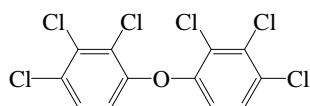
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: average $t_{1/2} = 55$ d in salmon for pentachloro-DPE congeners (Zitko & Carson 1977, Niimi 1986)

biological $t_{1/2} \sim 113$ d (range 81–144 d) in rainbow trout (average value for pentachloro-DPE congeners, Niimi 1986);

$t_{1/2} = 15$ d for Cl_4 -DPE to Cl_5 -DPE in waterborne exposed salmon and $t_{1/2} = 55$ d for diet-exposed fish (Niimi et al. 1994).

10.1.4.18 2,2',3,3',4,4'-Hexachlorodiphenyl ether (PCDE-128)

Common Name: 2,2',3,3',4,4'-Hexachlorodiphenyl ether

Synonym: PCDE-128

Chemical Name: 2,2',3,3',4,4'-hexachlorodiphenyl ether

CAS Registry No: 71585-39-2

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

141–142 (Navalainen et al. 1994)

95 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.206 (mp at $95^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.73×10^{-3} ; 4.33×10^{-4} (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

2.73×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

8.71×10^{-5} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

12.02 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.82 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.13 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

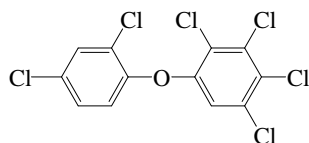
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: biological $t_{1/2} > 170$ d (range 100 to > 300 d) in rainbow trout (average value for hexachloro-DPE congeners, Niimi 1986)

10.1.4.19 2,2',3,4,4',5-Hexachlorodiphenyl ether (PCDE-137)



Common Name: 2,2',3,4,4',5-Hexachlorodiphenyl ether

Synonym: PCDE-137

Chemical Name: 2,2',3,4,4',5-hexachlorodiphenyl ether

CAS Registry No: 71585-36-9

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

78–80 (Navalainen et al. 1994)

69 (Ruelle & Kesselring 1997)

80 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.285 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

1.85×10^{-3} ; 2.18×10^{-3} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.61×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1043/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

2.0×10^{-4} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

2.04×10^{-4} ; 5.80×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.17 - 4878/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.22 - 3837/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

54.95 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 11.09 - 2794/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.72, 6.83 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

7.11 (GC-RT correlation, Hackenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.37 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

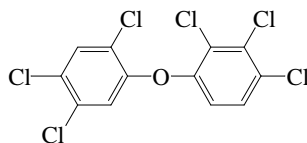
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 100$ d (range 69–179 d) in rainbow trout, mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.20 2,2',3,4,4',5'-Hexachlorodiphenyl ether (PCDE-138)



Common Name: 2,2',3,4,4',5'-Hexachlorodiphenyl ether

Synonym: PCDE-138

Chemical Name: 2,2',3,4,4',5'-hexachlorodiphenyl ether

CAS Registry No: 71585-38-1

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

69–70 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F :

0.359 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

1.84×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1014/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.70×10^{-4} (P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

1.73×10^{-4} ; 6.23×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/Pa) = 12.15 - 4866/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.21 - 3854/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

34.67 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa m^3/mol)] = 11.08 - 2840/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.01 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.01, 6.77 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.86 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

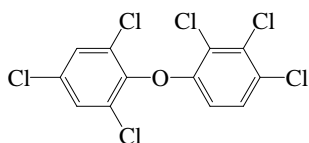
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 100$ d (range 69–179 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to >300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.21 2,2',3,4,4',6'-Hexachlorodiphenyl ether (PCDE-140)

Common Name: 2,2',3,4,4',6'-Hexachlorodiphenyl ether

Synonym: PCDE-140

Chemical Name: 2,2',3,4,4',6'-hexachlorodiphenyl ether

CAS Registry No: 106220-82-0

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

120–122 (Navalainen et al. 1994)

121 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.114 (mp at $121^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.99×10^{-3} ; 6.4×10^{-4} (quoted exptl., calculated-molar volume and mp, Ruelle & Kesselring 1997)

2.99×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

2.69×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

33.88 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.76 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.51 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

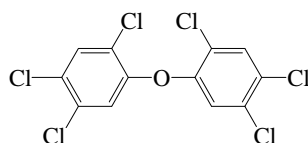
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 149$ d (range 99–302 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.22 2,2',4,4',5,5'-Hexachlorodiphenyl ether (PCDE-153)



Common Name: 2,2',4,4',5,5'-Hexachlorodiphenyl ether

Synonym: PCDE-153

Chemical Name: 2,2',4,4',5,5'-hexachlorodiphenyl ether

CAS Registry No: 71859-30-8

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

113–115 (Navalainen et al. 1994)

114 (Ruelle & Kesselring 1997)

115 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997; quoted, Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.134 (mp at $114^{\circ}C$)

0.126 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

1.65×10^{-4} ; 7.52×10^{-4} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.65×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1047/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.47×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

3.74×10^{-4} ; 4.71×10^{-5} (quoted supercooled liquid P_L from Hinckley et al. 1998; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.19 - 4916/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.24 - 3771/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

79.43 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log (H/(Pa m^3/mol)) = 11.11 - 2724/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.72 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.72, 6.84 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.21 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B :

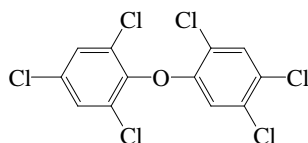
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 167$ d (range 98–553 d) in rainbow trout ; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.23 2,2',4,4',5,6'-Hexachlorodiphenyl ether (PCDE-154)



Common Name: 2,2',4,4',5,6'-Hexachlorodiphenyl ether

Synonym: PCDE-154

Chemical Name: 2,2',4,4',5,6'-hexachlorodiphenyl ether

CAS Registry No: 106220-81-9

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

94–96 (Navalainen et al. 1994)

95 (Ruelle & Kesselring 1997)

96 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997); quoted Passivirta et al. 1999

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.206 (mp at $95^{\circ}C$)

0.198 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

3.44×10^{-3} ; 1.16×10^{-3} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

3.44×10^{-3} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1090/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

6.46×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

6.64×10^{-4} ; 1.32×10^{-4} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.10 - 4760/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.15 - 4465/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

70.79 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 11.02 - 2582/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.49 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

6.49, 6.93 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.03 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

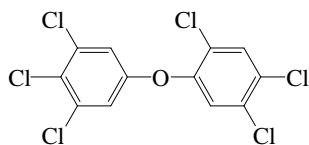
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 142$ d (range 90–330 d) in rainbow trout; mean $t_{1/2} > 170$ d (range 100 to > 300 d) for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.24 2,3',4,4',5,5'-Hexachlorodiphenyl ether (PCDE-167)



Common Name: 2,3',4,4',5,5'-Hexachlorodiphenyl ether

Synonym: PCDE-167

Chemical Name: 2,3',4,4',5,5'-hexachlorodiphenyl ether

CAS Registry No: 131138-20-0

Molecular Formula: $C_{12}H_4Cl_6O$

Molecular Weight: 376.878

Melting Point ($^{\circ}C$):

104–105 (Navalainen et al. 1994)

84 (Ruelle & Kesselring 1997)

105 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

321.0 (calculated-Le Bas method at normal boiling point)

244.0 (Ruelle & Kesselring 1997; quoted Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F :

0.161 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

7.18×10^{-4} ; 1.51×10^{-3} (quoted exptl., calculated-molar volume, MP and mobile order thermodynamics, Ruelle & Kesselring 1997)

7.18×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -1.868 - 1117/(T/K)$ (liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at 25 and reported temperature dependence equations $^{\circ}C$):

2.29×10^{-4} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

2.49×10^{-4} ; 4.0×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/Pa) = 12.20 - 4938/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.25 - 3822/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

120.23 (calculated-P/C, Kurz & Ballschmiter 1997)

$\log [H/(Pa\ m^3/mol)] = 11.12 - 2705/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.11 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.11, 6.99 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.42 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

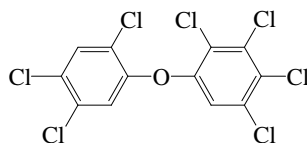
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} > 170$ d (range 100 to > 300 d) in rainbow trout for hexachlorodiphenyl ethers (Niimi 1986).

10.1.4.25 2,2',3,4,4',5,5'-Heptachlorodiphenyl ether (PCDE-180)



Common Name: 2,2',3,4,4',5,5'-Heptachlorodiphenyl ether

Synonym: PCDE-180

Chemical Name: 2,2',3,4,4',5,5'-heptachlorodiphenyl ether

CAS Registry No: 83992-69-2

Molecular Formula: $C_{12}H_3Cl_7O$

Molecular Weight: 411.324

Melting Point ($^{\circ}C$):

88–90 (Navalainen et al. 1994; quoted, Passivirta et al. 1999)

89 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

341.9 (calculated-Le Bas method at normal boiling point)

256.9 (Ruelle & Kesselring 1997; Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.236 (mp at $89^{\circ}C$)

0.227 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

1.30×10^{-4} ; 4.83×10^{-4} (quoted exptl.; calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

1.30×10^{-4} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

$\log [S_L/(mol/L)] = -2.344 - 1073/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

6.31×10^{-6} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

5.14×10^{-5} ; 1.17×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.31 - 5117/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.36 - 4046/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

199.53 (calculated-P/C, Kurz & Ballschmiter 1999)

$\log [H/(Pa \cdot m^3/mol)] = 11.70 - 2973/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.46 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

7.46, 7.20 (quoted lit., calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

7.39 (GC-RT correlation, Hankenberg et al. 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.55 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, log BCF or log K_B :

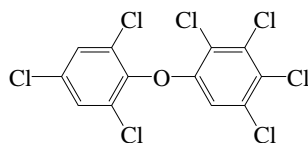
Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 146$ d (range 90–380 d) in rainbow trout; mean $t_{1/2} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);
 $t_{1/2} = 6$ –13 d for Cl₇-DPEs to Cl₇-DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.26 2,2',3,4,4',5,6'-Heptachlorodiphenyl ether (PCDE-182)



Common Name: 2,2',3,4,4',5,6'-Heptachlorodiphenyl ether

Synonym: PCDE-182

Chemical Name: 2,2',3,4,4',5,6'-heptachlorodiphenyl ether

CAS Registry No: 88467-63-4

Molecular Formula: $C_{12}H_3Cl_7O$

Molecular Weight: 411.324

Melting Point ($^{\circ}C$):

136–138 (Navalainen et al. 1994)

136 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

341.9 (calculated-Le Bas method at normal boiling point)

256.9 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.076 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.344 - 1215/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.01×10^{-4} ; 7.66×10^{-6} (supercooled liquid P_L , GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.35 - 5188/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.49 - 3976/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$):

$\log [H/(Pa \cdot m^3/mol)] = 11.74 - 2761/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.50 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

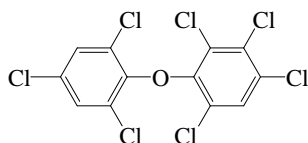
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean $t_{1/2} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);

$t_{1/2} = 6$ –13 d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.27 2,2',3,4,4',6,6'-Heptachlorodiphenyl ether (PCDE-184)



Common Name: 2,2',3,4,4',6,6'-Heptachlorodiphenyl ether

Synonym: PCDE-184

Chemical Name: 2,2',3,4,4',6,6'-heptachlorodiphenyl ether

CAS Registry No: 106220-84-2

Molecular Formula: $C_{12}H_3Cl_7O$

Molecular Weight: 411.324

Melting Point ($^{\circ}C$):

142 (calculated, Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

341.9 (calculated-Le Bas method at normal boiling point)

256.9 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.080 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.344 - 1227/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.32×10^{-4} ; 1.06×10^{-5} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F, Passivirta et al. 1999)

$\log (P_S/Pa) = 12.73 - 5858/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.78 - 4633/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

$\log [H/(Pa \cdot m^3/mol)] = 12.12 - 3406/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.53 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

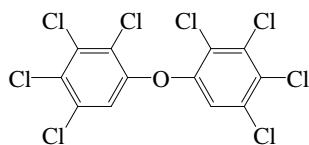
Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean $t_{1/2} > 300$ d (range 146 to > 300 d) for heptachlorodiphenyl ethers (Niimi 1986);

$t_{1/2} = 6-13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.28 2,2',3,3',4,4',5,5'-Octachlorodiphenyl ether (PCDE-194)



Common Name: 2,2',3,3',4,4',5,5'-Octachlorodiphenyl ether

Synonym: PCDE-194

Chemical Name: 2,2',3,3',4,4',5,5'-octachlorodiphenyl ether

CAS Registry No:

Molecular Formula: $C_{12}H_2Cl_8O$

Molecular Weight: 445.769

Melting Point ($^{\circ}C$):

125–128 (Navalainen et al. 1994)

126 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

362.8 (calculated-Le Bas method at normal boiling point)

269.8 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.102 (mp at $126^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3.30×10^{-5} ; 7.57×10^{-5} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

3.30×10^{-5} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

1.74×10^{-5} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

234.42 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.78 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.80 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

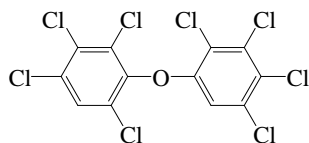
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.29 2,2',3,3',4,4',5,6'-Octachlorodiphenyl ether (PCDE-196)



Common Name: 2,2',3,3',4,4',5,6'-Octachlorodiphenyl ether

Synonym: PCDE-196

Chemical Name: 2,2',3,3',4,4',5,6'-octachlorodiphenyl ether

CAS Registry No: 85918-38-3

Molecular Formula: $C_{12}H_2Cl_8O$

Molecular Weight: 445.769

Melting Point ($^{\circ}C$):

147–149 (Navalainen et al. 1994)

149 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

362.8 (calculated-Le Bas method at normal boiling point)

269.8 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56.5 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.0595 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.819 - 1247/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

8.86×10^{-6} ; 5.27×10^{-6} (supercooled liquid P_L , GC-RT correlation; converted to solid P_s with fugacity ratio F, Passivirta et al. 1999)

$\log (P_s/Pa) = 12.57 - 5586/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.62 - 4341/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

$\log [H/(Pa \cdot m^3/mol)] = 12.44 - 3094/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.88 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

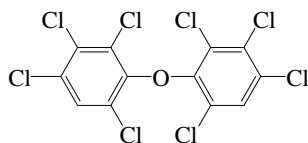
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.30 2,2',3,3',4,4',6,6'-Octachlorodiphenyl ether (PCDE-197)



Common Name: 2,2',3,3',4,4',6,6'-Octachlorodiphenyl ether

Synonym: PCDE-197

Chemical Name: 2,2',3,3',4,4',6,6'-octachlorodiphenyl ether

CAS Registry No: 117948-62-6

Molecular Formula: $C_{12}H_2Cl_8O$

Molecular Weight: 445.769

Melting Point ($^{\circ}C$):

124–126 (Navalainen et al. 1994)

126 (Passivirta et al. 1999)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

362.8 (calculated-Le Bas method at normal boiling point)

269.8 (Passivirta et al. 1999)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56.6 (estimated, Passivirta et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F :

0.100 (calculated, Passivirta et al. 1999)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ and reported temperature dependence equations):

$\log [S_L/(mol/L)] = -2.819 - 1179/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.75×10^{-5} ; 1.75×10^{-6} (supercooled liquid P_L , GC-RT correlation; converted to solid P_S with fugacity ratio F , Passivirta et al. 1999)

$\log (P_S/Pa) = 12.47 - 5405/(T/K)$ (solid, Passivirta et al. 1999)

$\log (P_L/Pa) = 9.52 - 4228/(T/K)$ (supercooled liquid, Passivirta et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ and reported temperature dependence equations):

$\log [H/(Pa\ m^3/mol)] = 12.34 - 3049/(T/K)$ (Passivirta et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

7.73 (calculated from lit. $\log K_{OW}$ and estimated $\log S_L$, Passivirta et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

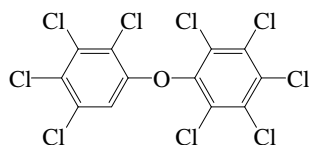
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13\ d$ for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.31 2,2',3,3',4,4',5,5',6-Nonachlorodiphenyl ether (PCDE-206)

Common Name: 2,2',3,3',4,4',5,5',6-Nonachlorodiphenyl ether

Synonym: PCDE-206

Chemical Name: 2,2',3,3',4,4',5,5',6-nonachlorodiphenyl ether

CAS Registry No: 83992-73-8

Molecular Formula: $C_{12}HCl_9O$

Molecular Weight: 480.214

Melting Point ($^{\circ}C$):

176–177 (Navalainen et al. 1994)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

383.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.704×10^{-6} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

6.92×10^{-6} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1949.84 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.07 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.08 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

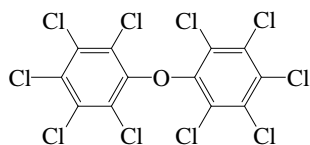
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 6 - 13$ d for Cl_7 -DPEs to Cl_9 -DPEs in various tissues of rat (Niimi et al. 1994).

10.1.4.32 Decachlorodiphenyl ether (PCDE-209)



Common Name: Decachlorodiphenyl ether

Synonym: PCDE-209

Chemical Name: decachlorodiphenyl ether

CAS Registry No: 31710-30-2

Molecular Formula: $C_{12}Cl_{10}O$

Molecular Weight: 514.659

Melting Point ($^{\circ}C$):

220–222 (Navalainen et al. 1994)

131 (Ruelle & Kesselring 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

404.6 (calculated-Le Bas method at normal boiling point)

295.6 (Ruelle & Kesselring 1997)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.64×10^{-8} ; 1.13×10^{-9} (quoted exptl., calculated-molar volume, mp and mobile order thermodynamics, Ruelle & Kesselring 1997)

5.64×10^{-8} (supercooled liquid, RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

1.58×10^{-6} (supercooled liquid P_L , GC-RT correlation, Kurz & Ballschmiter 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

14125 (calculated-P/C, Kurz & Ballschmiter 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

8.16 (RP-HPLC-RI correlation, Kurz & Ballschmiter 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.40 (calculated- K_{OW}/K_{AW} , Kurz & Ballschmiter 1999)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

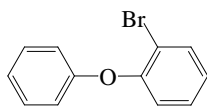
Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: mean biological $t_{1/2} = 46$ d (range 27–164 d) in rainbow trout (Niimi 1986)

10.1.5 BROMINATED DIPHENYL ETHERS

10.1.5.1 2-Bromodiphenyl ether (BDE-1)



Common Name: 2-Bromodiphenyl ether

Synonym: BDE-1, PBDE-1, 1-bromo-2-phenoxybenzene, 2-bromophenyl phenyl ether, *o*-bromophenyl phenyl ether

Chemical Name: 2-monobromodiphenyl ether

CAS Registry No: 7025-06-1

Molecular Formula: $C_{12}H_9BrO$

Molecular Weight: 249.103

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

63.7 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.163; 0.163 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3327/(T/K) + 10.37$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.24; 7.34 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: first-order degradation $t_{1/2} = 50$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first-order degradation $t_{1/2} = 900$ h (estimated by EPIWIN, Wania & Dugani 2003)

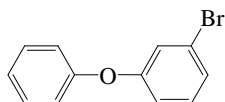
Ground water:

Sediment: first-order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first-order degradation $t_{1/2} = 900$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

10.1.5.2 3-Bromodiphenyl ether (BDE-2)



Common Name: 3-Bromodiphenyl ether

Synonym: BDE-2, PBDE-2, 1-bromo-3-phenoxybenzene, *m*-bromophenyl phenyl ether, 3-bromophenyl phenyl ether, 3-phenoxybromobenzene, 3-phenoxyphenyl bromide, *m*-bromodiphenyl ether, *m*-phenoxybromobenzene, *m*-phenoxyphenyl bromide

Chemical Name: 3-monobromodiphenyl ether

CAS Registry No: 6876-00-2

Molecular Formula: C₁₂H₉BrO

Molecular Weight: 249.103

Melting Point (°C):

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

218.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

65.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):

0.128; 0.125 (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

log (P_L/Pa) = -3416/(T/K) + 10.56, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant (Pa·m³/mol at 25°C):

Octanol/Water Partition Coefficient, log K_{OW}:

Octanol/Air Partition Coefficient, log K_{OA}:

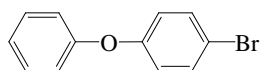
7.36; 7.44 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{OC}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

10.1.5.3 4-Bromodiphenyl ether (BDE-3)

Common Name: 4-Bromophenyl phenyl ether

Synonym: BDE-3, PBDE-3, *p*-bromophenyl phenyl ether, 1-bromo-4-phenoxybenzene, 4-bromophenyl phenyl ether, 4-phenoxybromobenzene, 4-phenoxyphenyl bromide, *p*-bromodiphenyl ether, *p*-bromophenoxybenzene, *p*-phenoxybromobenzene, *p*-phenoxyphenyl bromide

Chemical Name: 4-bromodiphenyl ether, bromophenyl ether

CAS Registry No: 101-55-3

Molecular Formula: $C_{12}H_9BrO$, $C_6H_5-O-C_6H_4Br$

Molecular Weight: 249.103

Melting Point ($^{\circ}C$):

18.72 (Weast 1977, 1982–83)

18.0 (Dean 1985, 1992)

Boiling Point ($^{\circ}C$):

310.1 (Weast 1977, 1982–83)

305 (Dean 1985, 1992)

Density (g/cm^3 at $20^{\circ}C$):

1.423 (Dean 1985)

Molar Volume (cm^3/mol):

154.8 ($20^{\circ}C$, Stephenson & Malanowski 1987)

218.9 (calculated-Le Bas method at normal boiling point)

175.1 (calculated-density)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

47.9 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.80 (calculated- K_{ow} , Mabey et al. 1982)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.20 ($20^{\circ}C$, calculated, Dreisbach 1952; quoted, Callahan et al. 1979; Mabey et al. 1982)

$\log(P_L/kPa) = 5.80633 - 1683.84/(-140.25 + T/K)$, temp range 463–673 K, (Antoine eq., Stephenson & Malanowski 1987)

0.259 (supercooled liquid PL, GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -2503/(T/K) + 7.81$, (Clausius-Clapeyron eq. from GC-RT correlation measurement, Tittlemier et al. 2002)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated):

10.13 (20 – $25^{\circ}C$, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.28 (calculated as per Leo et al. 1971 using data of Branson 1977, Callahan et al. 1979; quoted, Ryan et al. 1988)

4.94 (calculated, Mabey et al. 1982)

5.24 (quoted, Van Leeuwen et al. 1992)

4.85 (estimated, Tittlemier et al. 2002)

Bioconcentration Factor, log BCF:

4.114 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, log K_{OC} :

4.623 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $\ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $\ll 1.0 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982).

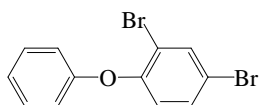
Hydrolysis:

Biodegradation: estimated half-life of 4.0 h in activated sludge, based on biodegradation of 4-chlorophenyl phenyl ether in activated sewage sludge (Branson 1978; quoted, Callahan et al. 1979).

Biotransformation: estimated rate constant of $3 \times 10^{-9} \text{ mL cell}^{-1} \text{ h}^{-1}$ for the bacterial transformation in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

Half-Lives in the Environment:

10.1.5.4 2,4-Dibromodiphenyl ether (BDE-7)

Common Name: 2,4-Dibromodiphenyl ether

Synonym: BDE-7, PBDE-7, 2,4-dibromo-1-phenoxybenzene

Chemical Name: 2,4-dibromodiphenyl ether

CAS Registry No: 171977-44-9

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

75.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0168; 0.0153 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3941/(T/K) + 11.34$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.03 (for dibromodiphenyl ethers, RP-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.37; 8.36 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

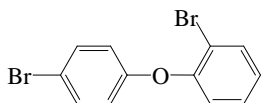
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.5 2,4'-Dibromodiphenyl ether (BDE-9)



Common Name: 2,4'-Dibromodiphenyl ether

Synonym: BDE-8, PBDE-8, 1-bromo-2-(4-bromophenoxy)-benzene

Chemical Name: 2,4'-dibromodiphenyl ether

CAS Registry No: 147217-71-8

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

76.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0137; 0.0124 (supercooled liquid P_L ; calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3991/(T/K) + 11.42$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

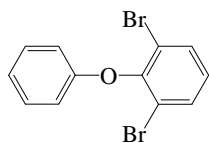
8.47; 8.45 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.6 2,6-Dibromodiphenyl ether (BDE-10)

Common Name: 2,6-Dibromodiphenyl ether

Synonym: BDE-10, PBDE-10, 1,3-dibromo-2-phenoxybenzene

Chemical Name: 2,6-dibromodiphenyl ether

CAS Registry No: 51930-04-2

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

73.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0277; 0.0256 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -3818/(T/K) + 11.25$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.03 (dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.12; 8.13 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

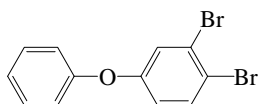
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.7 3,4-Dibromodiphenyl ether (BDE-12)



Common Name: 3,4-Dibromodiphenyl ether

Synonym: BDE-12, PBDE-12, 1,2-dibromo-4-phenoxybenzene

Chemical Name: 3,4-dibromodiphenyl ether

CAS Registry No: 189084-59-1

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0119; 0.107 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4020/(T/K) + 11.56$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

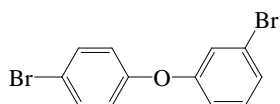
8.55; 8.52 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.8 3,4'-Dibromodiphenyl ether (BDE-13)

Common Name: 3,4'-Dibromodiphenyl ether

Synonym: BDE-13, PBDE-13, 1-bromo-3-(4-bromophenoxy)-benzene

Chemical Name: 3,4'-dibromodiphenyl ether

CAS Registry No: 83694-71-7

Molecular Formula: $C_{12}H_8Br_2O$

Molecular Weight: 327.999

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.0 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.0113; 0.0101 (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4044/(T/K) + 11.62$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (quoted value for dibromodiphenyl ether, Pijnenburg et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.57; 8.54 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

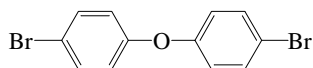
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.9 4,4'-Dibromodiphenyl ether (BDE-15)



Common Name: 4,4'-Dibromodiphenyl ether

Synonym: BDE-15, PBDE-15, 1,1-oxybis[4-bromo]benzene, bis(4-bromophenyl)ether, *p*, *p'*-dibromodiphenyl ether

Chemical Name: 4,4'-dibromodiphenyl ether

CAS Registry No: 2050-47-7

Molecular Formula: C₁₂H₈Br₂O

Molecular Weight: 327.999

Melting Point (°C):

57–58 (Tittlemier et al. 2002)

57.7 (Wania & Dugani 2003)

Boiling Point (°C):

Density (g/cm³):

Molar Volume (cm³/mol):

242.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.0 (Wong et al. 2001)

67.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

0.477 (mp at 57.5°C, Wania & Dugani 2003)

Water Solubility (g/m³ or mg/L at 25°C):

0.130 (generator column-GC/ECD, Tittlemier et al. 2002)

0.273, 0.79 (supercooled S_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at 25°C and reported temperature dependence equation):

0.0188–0.0127 (for dibromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

9.84 × 10⁻³; 8.80 × 10⁻³ (supercooled liquid P_L: calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

log (P_L/Pa) = -4074/(T/K) + 11.65, (GC-RT correlation, Wong et al. 2001)

0.0173 (supercooled liquid P_L, GC-RT correlation, Tittlemier et al. 2002)

log (P_L/Pa) = -3528/(T/K) + 10.08, (Clausius-Clapeyron equation from GC-RT correlation measurements, Tittlemier et al. 2002)

0.0143, 0.010 (supercooled, P_L, selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant (Pa·m³/mol at 25°C):

21 (calculated-P_L/C_L, Tittlemier et al. 2002)

4.11 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, log K_{OW}:

5.03 (for dibromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.03 (value for dibromodiphenyl ether, Pijnenburg et al. 1995)

5.55 (estimated, Tittlemier et al. 2002)

5.03, 5.48 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, log K_{OA}:

8.64; 8.60 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

8.79, 8.63 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photochemical degradation pathway of BDE15 undergoes strict debromination via first-order decay, $k = 1.98 \times 10^{-2} \text{ min}^{-1}$ in 100% CH_3CN and $k = 3.10 \times 10^{-2} \text{ min}^{-1}$ in CH_3OH , corresponding to $t_{1/2} \sim 30 \text{ min}$. (Rayne et al. 2003)

Photooxidation:

Hydrolysis:

Biodegradation: complete debromination under anaerobic microbial degradation in a fixed-film plug-flow bioreactor (Rayne et al. 2003)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 120 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

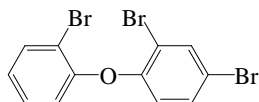
Ground water:

Sediment: first order degradation $t_{1/2} = 5760 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

10.1.5.10 2,2',4-Tribromodiphenyl ether (BDE-17)



Common Name: 2,2',4-Tribromodiphenyl ether

Synonym: PBDE-17

Chemical Name: 2,2',4-tribromodiphenyl ether

CAS Registry No: 147217-75-2

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)

0.00219 (supercooled P_L , GC-RT correlation on a CPSil-8 column, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of value for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

9.30* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -3.54 + 3803/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

9.966, 9.385, 8.841, 8.332 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

9.919, 9.339, 8.789, 8.290 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.10.1

Reported octanol-air partition coefficients of 2,2',4-tribromodiphenyl ether (PBDE 17) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
		QRSETP* model 3	
15	9.777	15	9.966
25	9.27	25	9.385
35	8.901	35	8.841
45	8.517	45	8.332
25	9.3	QRSETP model 5	
		15	9.919
		25	9.339
		35	8.798
		45	9.29
log K _{OA} = A + B/(T/K)			
A	-3.45		
B	3803		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 72.8$			

Quantitative relationships between structures, environmental temperatures and properties.

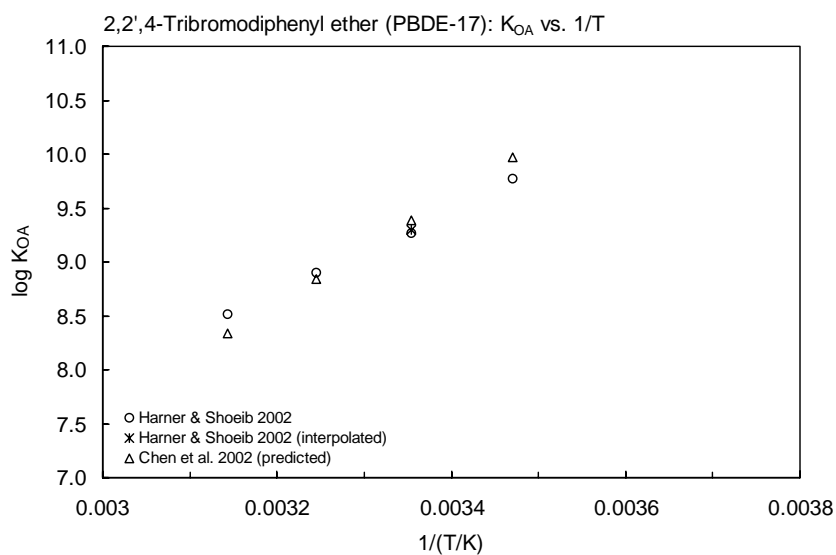
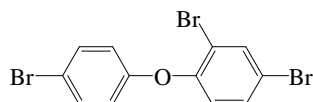


FIGURE 10.1.5.10.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4-tribromodiphenyl ether (PBDE-17).

10.1.5.11 2,4,4'-Tribromodiphenyl ether (BDE-28)



Common Name: 2,4,4'-Tribromodiphenyl ether

Synonym: PBDE-28, 2,4-dibromo-1-(4-bromophenoxy)-benzene, p-bromophenyl 2,4-dibromophenyl ether

Chemical Name: 2,4,4'-tribromodiphenyl ether

CAS Registry No: 41318-75-6

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

64–64.5 (Tittlemier et al. 2002)

64.25 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

94.05 (Tittlemier & Tomy 2001)

79.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.409 (at mp $64.25^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

0.070 (solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.173, 0.334 (supercooled liquid S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)

1.78×10^{-4} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -4912/(T/K) + 12.73$, (GC-RT correlation, Tittlemier & Tomy 2001)

0.00160 (supercooled P_L , GC-RT correlation on a CPSil-8 column, Wong et al. 2001)

2.19×10^{-3} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -4160/(T/K) + 11.30$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

1.96×10^{-3} , 1.57×10^{-3} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

5.1 (calculated- P_L/C_L , Tittlemier et al. 2002)

1.924 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

5.98 (estimated from PCDEs and fragment constant, Tittlemier et al. 2002)

5.53, 5.80 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

9.50* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -3.54 + 3889/(T/K)$, temp range 15–45°C (generator column-GC, Harner & Shoeib 2002)

10.279, 9.689, 9.154, 8.645 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)

10.213, 9.634, 9.092, 8.585 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

9.50, 9.41 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 0.019 \text{ d}^{-1}$ with $t_{1/2} = 36.5 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 128 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 5760 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 1440 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota: depuration $t_{1/2} = 36.5 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.11.1
Reported octanol-air partition coefficients of 2,4,4'-tribromodiphenyl ether (PBDE 28) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	9.994	15	10.279
25	9.46	25	9.698
35	9.077	35	9.154
45	8.709	45	8.645
25	9.5	QRSETP model 5	
		15	10.213
		25	9.634
		35	9.092
		45	8.585
$\log K_{OA} = A + B/(T/K)$			
A	-3.54		
B	3889		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 74.5$			

Quantitative relationships between structures, environmental temperatures and properties.

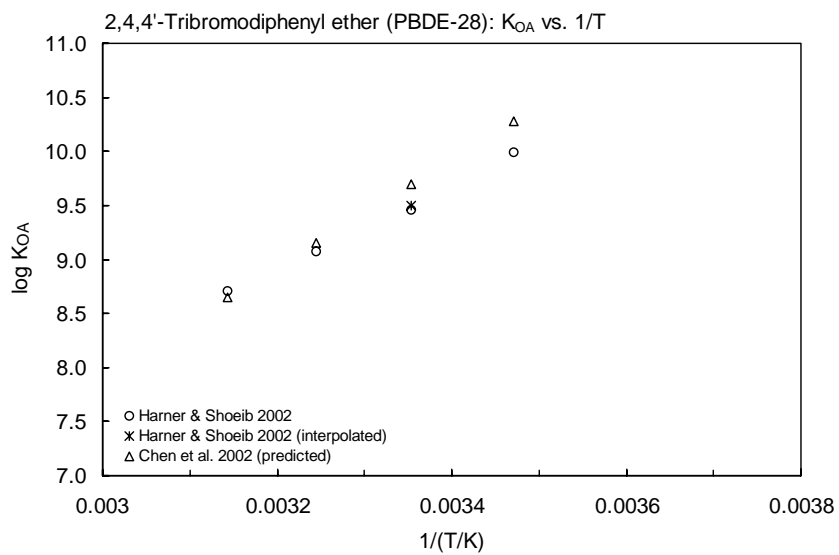
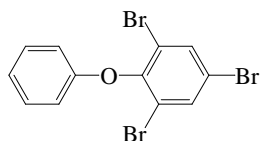


FIGURE 10.1.5.11.1 Logarithm of K_{OA} versus reciprocal temperature for 2,4,4'-tribromodiphenyl ether (PBDE-28).

10.1.5.12 2,4,6-Tribromodiphenyl ether (BDE-30)

Common Name: 2,4,6-Tribromodiphenyl ether

Synonym: PBDE-30, BDE-30, 1,3,5-tribromo-2-phenoxybenzene

Chemical Name: 2,4,6-tribromodiphenyl ether

CAS Registry No: 155999-95-4

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

85.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)

4.56×10^{-3} ; 3.96×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4232/(T/K) + 11.85$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.02; 8.94 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

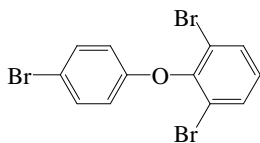
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.13 2,4',6-Tribromodiphenyl ether (BDE-32)



Common Name: 2,4',6-Tribromodiphenyl ether

Synonym: PBDE-32, BDE-32, 1,3-dibromo-2-(4-bromophenoxy)-benzene

Chemical Name: 2,4',6-tribromodiphenyl ether

CAS Registry No: 189083-60-4

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

83.3 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for triBDE, Alcock et al. 1999)

2.25×10^{-3} ; 1.90×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4352/(T/K) + 11.94$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.59 (quoted values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

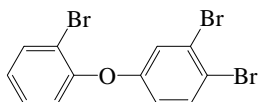
9.28; 9.18 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.14 2',3,4-Tribromodiphenyl ether (BDE-33)

Common Name: 2',3,4-Tribromodiphenyl ether

Synonym: PBDE-33, BDE-33. 1,2-dibromo-4-(2-bromophenoxy)-benzene

Chemical Name: 2',3,4-tribromodiphenyl ether

CAS Registry No: 147217-78-5

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

81.0 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.01150 (estimated for tri-BDE, Alcock et al. 1999)

1.78×10^{-3} ; 1.49×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4443/(T/K) + 12.15$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

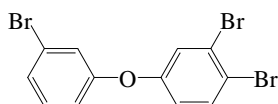
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.15 3,3',4-Tribromodiphenyl ether (BDE-35)



Common Name: 3,3',4-Tribromodiphenyl ether

Synonym: PBDE-35, BDE-35, 1,2-dibromo-4-(4-bromophenoxy)-benzene

Chemical Name: 3,3',4-tribromodiphenyl ether

CAS Registry No: 147217-80-9

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.4 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for triBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00155 (estimated for triBDE, Alcock et al. 1999)

1.39×10^{-3} ; 1.15×10^{-3} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4512/(T/K) + 12.28$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of values for tribromodiphenyl ethers, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

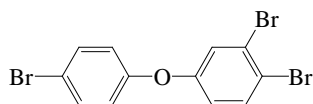
9.61; 9.48 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.16 3,4,4'-Tribromodiphenyl ether (BDE-37)

Common Name: 3,4,4'-Tribromodiphenyl ether

Synonym: PBDE-37, BDE-37, 1,2-dibromo-4-(4-bromophenoxy)-benzene

Chemical Name: 3,4,4'-tribromodiphenyl ether

CAS Registry No: 147217-81-0

Molecular Formula: $C_{12}H_7Br_3O$

Molecular Weight: 406.895

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

265.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

86.7 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00038 (calculated for tri-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

0.00266–0.00150 (for tribromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.00266–0.00150 (estimated for tri-BDE, Alcock et al. 1999)

1.02×10^{-3} ; 8.0×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4528/(T/K) + 12.20$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.47–5.58 (for tribromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.47–5.58 (quoted range of values for tribromodiphenyl ether, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.68; 9.54 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

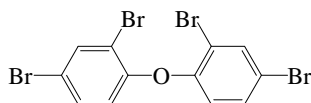
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.17 2,2',4,4'-Tetrabromodiphenyl ether (BDE-47)



Common Name: 2,2',4,4'-Tetrabromodiphenyl ether

Synonym: PBDE-47, BDE-47, 1,1'-oxybis[2,4-dibromo-benzene], NSC 21724

Chemical Name: 2,2',4,4'-tetrabromodiphenyl ether

CAS Registry No: 5436-43-1

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

83.5–84.5 (Tittlemier et al. 2002)

84.0 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

103.13 (Tittlemier & Tomy 2001)

92.0 (Wong et al. 2001)

94.6 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.261 (calculated at mp $84^{\circ}C$, Wania & Dugani 2002)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetra-BDE, Alcock et al. 1999)

0.015 (solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.0496, 0.0947 (supercooled liquid S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

2.19×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5386/(T/K) + 13.42$, (GC-RT correlation, Tittlemier & Tomy 2001)

3.19×10^{-4} ; 2.50×10^{-4} (supercooled P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4805/(T/K) + 12.62$, (GC-RT correlation, Wong et al. 2001)

1.86×10^{-4} (supercooled liquid P_L , GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -4940/(T/K) + 12.85$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

2.66×10^{-4} , 2.15×10^{-4} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.5 (calculated-P/C, Tittlemier et al. 2002)

1.107 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.02 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)

6.55 (estimated, Tittlemier et al. 2002)

6.11, 6.39 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

10.53* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -6.47 + 5068/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)

10.987, 10.406, 9.863, 9.353 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)

10.928, 10.349, 9.807, 9.300 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

10.34; 10.14 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

10.53, 10.44 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 120 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt}$, $k_2 = 0.090 \text{ d}^{-1}$ in blue mussels (Gustafsson et al. 1999)

$k_1 = 0.108 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$ in Lake Höytiäinen sediment; $0.251 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$ in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

$k_2 = 0.034 \text{ d}^{-1}$ in Lake Höytiäinen sediment; 0.071 d^{-1} in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

$k_2 = 0.023 \text{ d}^{-1}$ with $t_{1/2} = 30.1 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 256 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota: depuration half-life of 7.7 d in blue mussels (Gustafsson et al. 1999);

biphasic depuration kinetics observed in oligochaete tissues with half-life of 10.5–47.5 h in compartment A for sediment ingesting oligochaetes (Leppänen & Kukkonen 2004)

depuration $t_{1/2} = 30.1 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.17.1

Reported octanol-air partition coefficients of 2,2',4,4'-tetrabromodiphenyl ether (PBDE 47) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
15	11.129	15	10.987
25	10.499	25	10.406
35	10.063	35	9.863
45	9.428	45	9.353
25	10.53	QRSETP model 5	
		15	10.928
		25	10.349
		35	9.807
		45	9.3
log K _{OA} = A + B/(T/K)			
A	-6.47		
B	5068		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 97.0$			

Quantitative relationships between structures, environmental temperatures and properties.

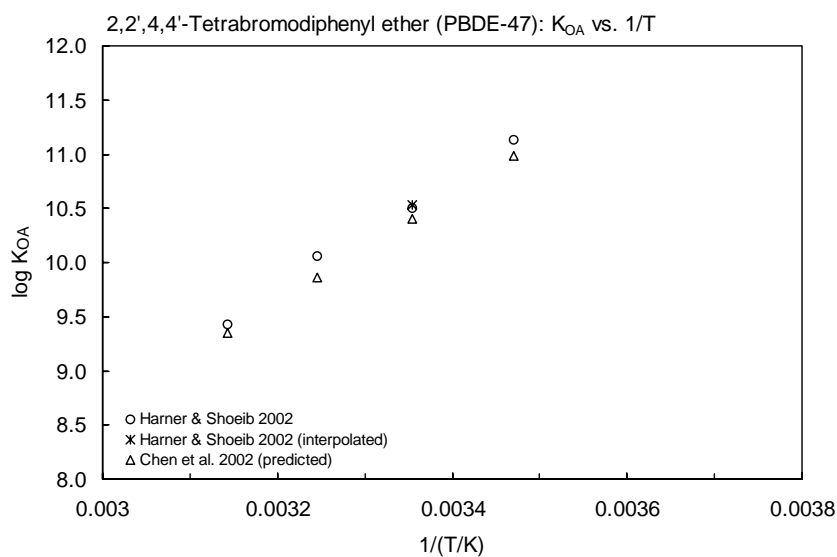
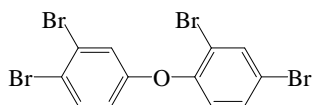


FIGURE 10.1.5.17.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4'-tetrabromodiphenyl ether (PBDE-47).

10.1.5.18 2,3',4,4'-Tetrabromodiphenyl ether (BDE-66)

Common Name: 2,3',4,4'-Tetrabromodiphenyl ether

Synonym: PBDE-66, BDE-66, 1,2-dibromo-4-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,3',4,4'-tetrabromodiphenyl ether

CAS Registry No: 189084-61-5

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

93.5 (Wong et al. 2001)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetraBDE, Alcock et al. 1999)

0.018 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

2.38×10^{-4} ; 1.90×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4882/(T/K) + 12.75$, (GC-RT correlation, Wong et al. 2001)

1.22×10^{-4} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5109/(T/K) + 13.23$, (Clausius-Clapeyron eq. form GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.50 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.73 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

10.82* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -7.88 + 5576/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

11.348, 10.767, 10.223, 9.714 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

11.281, 10.702, 10.161, 9.653 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

10.49; 10.28 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.18.1
Reported octanol-air partition coefficients of 2,3',4,4'-tetrabromodiphenyl ether (PBDE 66) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^{\circ}\text{C}$	log K_{OA}	$t/^{\circ}\text{C}$	log K_{OA}
QRSETP* model 3			
15	11.516	15	11.348
25	10.773	25	10.767
35	10.224	35	10.223
45	9.673	45	9.714
25	10.82	QRSETP model 5	
		15	11.281
		25	10.702
		35	10.161
		45	9.653
log $K_{OA} = A + B/(T/K)$			
A	-7.88		
B	5576		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 107.0$			

Quantitative relationships between structures, environmental temperatures and properties.

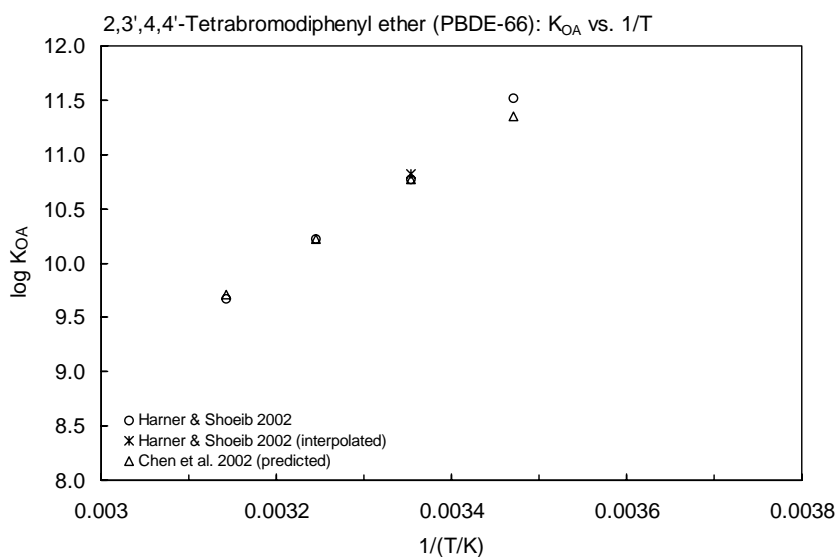
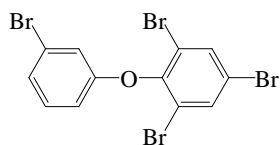


FIGURE 10.1.5.18.1 Logarithm of K_{OA} versus reciprocal temperature for 2,3',4,4'-tetrabromodiphenyl ether (PBDE-66).

10.1.5.19 2,3',4,6-Tetrabromodiphenyl ether (BDE-69)

Common Name: 2,3',4,6-Tetrabromodiphenyl ether

Synonym: PBDE-69, BDE-69, 1,3,5-tribromo-2-(30bromophenoxy)-benzene

Chemical Name: 2,3',4,6-tetrabromodiphenyl ether

CAS Registry No: 327185-09-1

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

91.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetraBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

4.0×10^{-4} ; 3.20×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4757/(T/K) + 12.56$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.23; 10.04 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

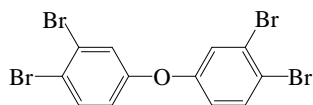
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.20 3,3',4,4'-Tetrabromodiphenyl ether (BDE-77)



Common Name: 3,3',4,4'-Tetrabromodiphenyl ether

Synonym: PBDE-77, BDE-77, 1,1'-xylbix[2,3-dibromophenoxy]-benzene

Chemical Name: 3,3',4,4'-tetrabromodiphenyl ether

CAS Registry No: 93703-48-1

Molecular Formula: $C_{12}H_6Br_4O$

Molecular Weight: 485.791

Melting Point ($^{\circ}C$):

96.7–98 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

288.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

95.3 (Wong et al. 2001)

98.7 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.00007 (calculated for tetraBDE, Alcock et al. 1999)

0.006 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

3.35×10^{-4} – 2.60×10^{-4} (for tetrabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

1.56×10^{-4} ; 1.20×10^{-4} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -4977/(T/K) + 12.89$, (GC-RT correlation, Wong et al. 2001)

6.79×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5156/(T/K) + 13.13$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.2 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.87–6.16 (for tetrabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

5.87–6.16 (quoted range for tetra-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.96 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

10.87* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -5.69 + 4936/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

11.343, 10.762, 10.218, 9.709 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

11.218, 10.603, 10.097, 9.590 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

10.70; 10.46 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.20.1

Reported octanol-air partition coefficients of 3,3',4,4'-tetrabromodiphenyl ether (PBDE 77) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^{\circ}\text{C}$	log K_{OA}	$t/^{\circ}\text{C}$	log K_{OA}
QRSETP* model 3			
15	11.486	15	11.343
25	10.829	25	10.762
35	10.371	35	10.218
45	9.844	45	9.709
25	10.87	QRSETP model 5	
log $K_{OA} = A + B/(T/K)$		15	11.218
A	-5.69	25	10.639
B	4936	35	10.097
enthalpy of phase change		45	9.59
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 94.5$			

Quantitative relationships between structures, environmental temperatures and properties.

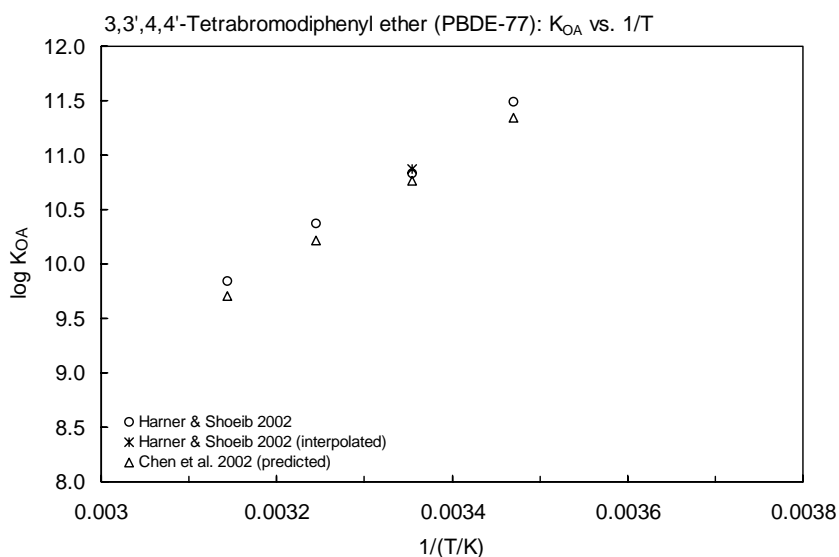
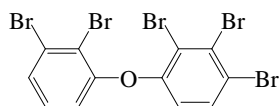


FIGURE 10.1.5.20.1 Logarithm of K_{OA} versus reciprocal temperature for 3,3',4,4'-tetrabromodiphenyl ether (PBDE-77).

10.1.5.21 2,2',3,3',4-Pentabromodiphenyl ether (BDE-82)



Common Name: 2,2',3,3',4-Pentabromodiphenyl ether

Synonym: PBDE-82, BDE-82, 1,2,3-tribromo-4-(2,3-dibromophenoxy)-benzene

Chemical Name: 2,2',3,3',4-pentabromodiphenyl ether

CAS Registry No: 327185-11-5

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

99.1 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for pentaBDE, Alcock et al. 1999)

6.47×10^{-5} ; 4.80×10^{-5} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5175/(T/K) + 13.12$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.14; 10.86 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

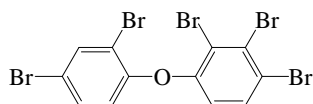
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.22 2,2',3,4,4'-Pentabromodiphenyl ether (BDE-85)



Common Name: 2,2',3,4,4'-Pentabromodiphenyl ether

Synonym: PBDE-85, BDE-85, 1,2,3-tribromo-4-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,2',3,4,4'-pentabromodiphenyl ether

CAS Registry No: 182346-21-0

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

119–121 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

110.95 (Tittlemier & Tomy 2001)

110 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

0.006 (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for pentaBDE, Alcock et al. 1999)

2.88×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5795/(T/K) + 13.91$, (GC-RT correlation, Tittlemier & Tomy 2001)

2.81×10^{-5} (supercooled P_L , GC-RT correlation on a CPSil-8 column, Wong et al. 2001)

9.86×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5761/(T/K) + 14.43$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.11 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

7.03 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.66* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

12.312, 11.631, 11.118, 10.544 (15 , 25 , 35 , $45^{\circ}C$, generator column-GC/MS, Harner & Shoeib 2002)

$\log K_{OA} = -6.22 + 5331/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

12.131, 11.549, 11.006, 10.497 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

12.130, 11.551, 11.009, 10.502 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.22.1

Reported octanol-air partition coefficients of 2,2',3,4,4'-pentabromodiphenyl ether (PBDE 85) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	12.312	15	12.131
25	11.631	25	11.549
35	11.118	35	11.006
45	10.544	45	10.497
25	11.66	QRSETP model 5	
		15	12.13
		25	11.551
		35	11.009
		45	10.502
log $K_{OA} = A + B/(T/K)$			
A	-6.22		
B	5331		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 102.0$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

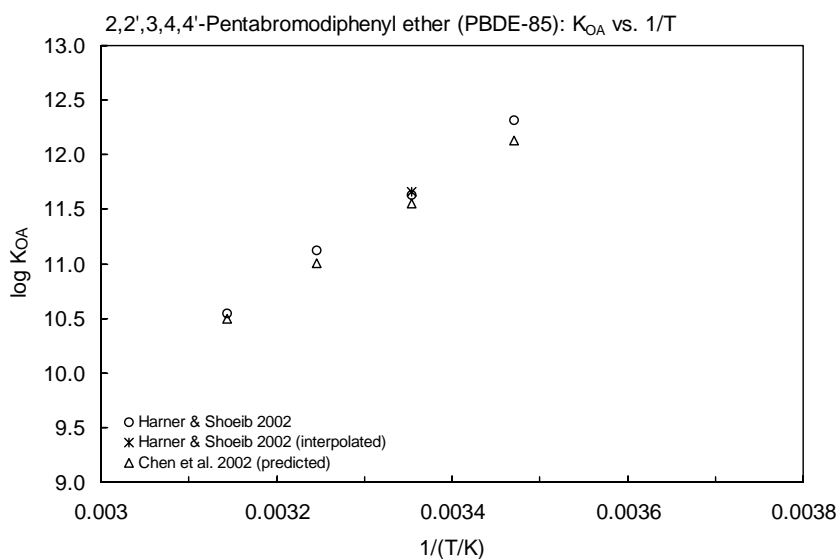
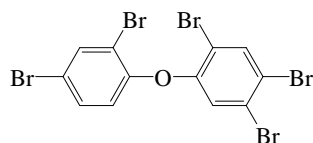


FIGURE 10.1.5.22.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',3,4,4'-pentabromodiphenyl ether (PBDE-85).

10.1.5.23 2,2',4,4',5-Pentabromodiphenyl ether (BDE-99)



Common Name: 2,2',4,4',5-Pentabromodiphenyl ether

Synonym: PBDE-99, BDE-99, 1,2,4-tribromo-5-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,2',4,4',5-pentabromodiphenyl ether

CAS Registry No: 60348-60-9

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

90.5–94.5 (Tittlemier et al. 2002)

92.5 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

104.80 (Tittlemier & Tomy 2001)

100.2 (Wong et al. 2001)

108 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.215 (at mp $92.5^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

0.0094 (solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.0275, 0.0389 (supercooled S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for pentaBDE, Alcock et al. 1999)

1.26×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5474/(T/K) + 13.47$, (GC-RT correlation, Tittlemier & Tomy 2001)

6.82×10^{-5} ; 5.0×10^{-5} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5241/(T/K) + 13.41$, (GC-RT correlation, Wong et al. 2001)

1.76×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5339/(T/K) + 13.37$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

4.57×10^{-5} , 3.63×10^{-5} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.23 (calculated- P_L/C_L , Tittlemier et al. 2002)

0.530 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (for pentabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

- 6.81 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)
 7.13 (estimated, Tittlemier et al. 2002)
 6.61, 6.76 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.
 Additional data at other temperatures designated * are compiled at the end of this section:

- 11.31* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)
 $\log K_{OA} = -4.64 + 4757/(T/K)$, temp range: 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)
 12.067, 11.485, 10.942, 10.433 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)
 12.002, 11.422, 10.881, 10.373 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)
 11.28; 10.99 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)
 11.31, 11.26 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (K_1 and K_2):

- $k_1 = 170 \text{ L d}^{-1} \text{ g}^{-1} \text{ dry wt}$; $k_2 = 0.123 \text{ d}^{-1}$ in blue mussels (Gustafsson et al. 1999)
 $k_1 = 0.066 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$; $k_2 = 0.022 \text{ d}^{-1}$ in Lake Höytiäinen sediment; $k_1 = 0.99 \text{ g org. C g}^{-1} \text{ lipid h}^{-1}$;
 $k_2 = 0.026 \text{ d}^{-1}$ in Lake Kuorinka sediment (sediment ingesting oligochaetes, Leppänen & Kukkonen 2004)

Half-Lives in the Environment:

- Air: first order degradation $t_{1/2} = 467 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Ground water:
 Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)
 Biota: depuration $t_{1/2} = 5.6 \text{ d}$ in blue mussels (Gustafsson et al. 1999);
 biphasic depuration kinetics observed in oligochaete tissues with $t_{1/2} = 10.5\text{--}47.5 \text{ h}$ in compartment A for sediment ingesting oligochaetes (Leppänen & Kukkonen 2004)

TABLE 10.1.5.23.1

Reported octanol-air partition coefficients of 2,2',4,4',5-pentabromodiphenyl ether (PBDE 99) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
		QRSETP* model 3	
15	11.847	15	12.067
25	11.321	25	11.485
35	10.887	35	10.942
45	10.258	45	10.433
25	11.31	QRSETP model 5	
		15	12.002
		25	11.422
		35	10.881
		45	10.373
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 91.1$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

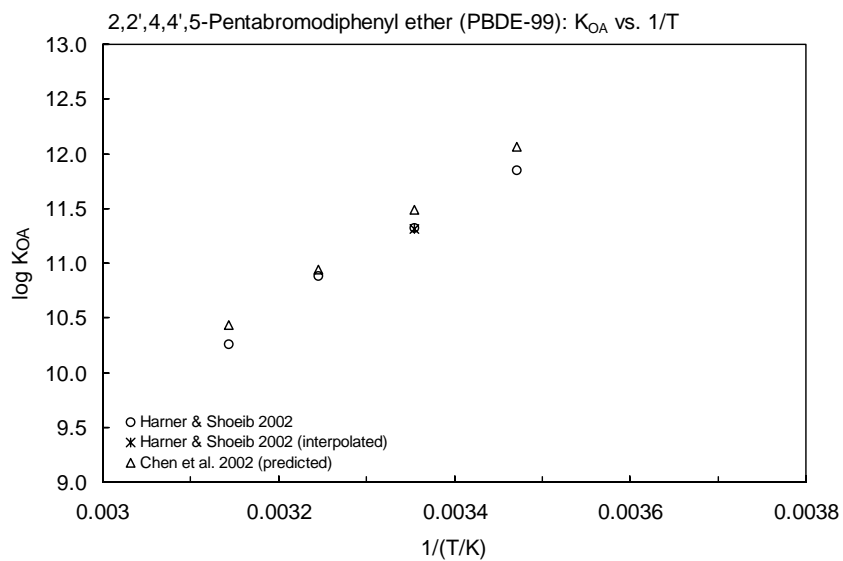
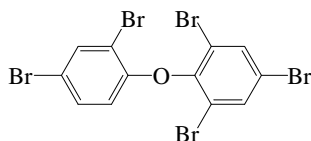


FIGURE 10.1.5.23.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',5-pentabromodiphenyl ether (PBDE-99).

10.1.5.24 2,2',4,4',6-Pentabromodiphenyl ether (BDE-100)



Common Name: 2,2',4,4',6-Pentabromodiphenyl ether

Synonym: PBDE-100, 1,3,5-tribromo-2-(2,4-dibromophenoxy)-benzene

Chemical Name: 2,2',4,4',6-pentabromodiphenyl ether

CAS Registry No: 189084-64-8

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

102 (Tittlemier et al. 2002)

110 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

102 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.179 (at mp $100.5^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.040 (generator column-GC/ECD, Tittlemier et al. 2002)

0.0499, 0.0541 (supercooled S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

2.86×10^{-5} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5339/(T/K) + 13.37$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

3.99×10^{-5} , 3.68×10^{-5} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.069 (calculated- P_L/C_L , Tittlemier et al. 2002)

0.384 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

6.86 (estimated, Tittlemier et al. 2002)

6.51, 6.53 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.13* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -7.18 + 5459/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

11.721, 11.140, 10.596, 10.087 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

11.758, 11.179, 10.637, 10.130 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

11.20; 11.52 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

11.13, 11.02 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 357$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

TABLE 10.1.5.24.1

Reported octanol-air partition coefficients of 2,2',4,4',6-pentabromodiphenyl ether (PBDE 100) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^{\circ}\text{C}$	log K_{OA}	$t/^{\circ}\text{C}$	log K_{OA}
		QRSETP* model 3	
15	11.755	15	11.721
25	11.185	25	11.14
35	10.509	35	10.596
45	9.993	45	10.087
25	11.13	QRSETP model 5	
		15	11.758
		25	11.179
		35	10.637
		45	10.13
log $K_{OA} = A + B/(T/K)$			
A	-7.18		
B	5459		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 105.0$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

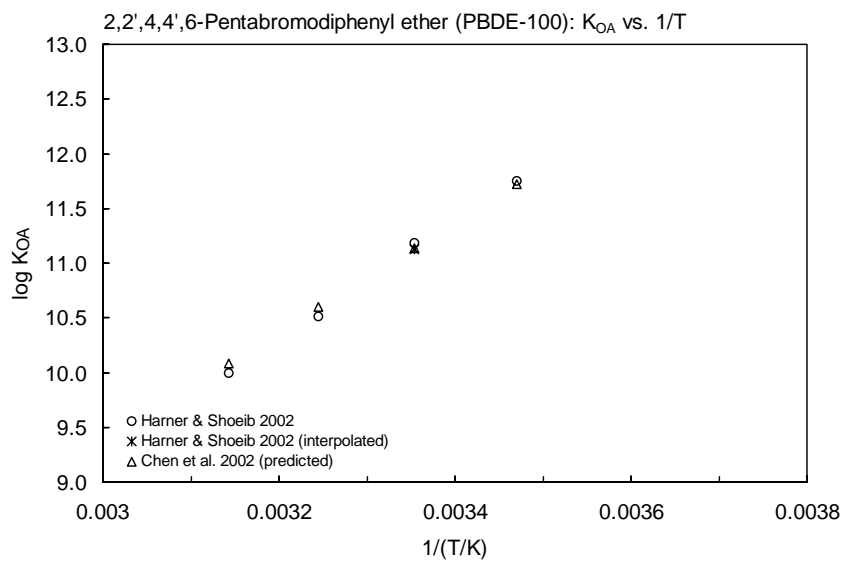
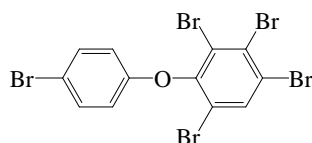


FIGURE 10.1.5.24.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',6-pentabromodiphenyl ether (PBDE-100).

10.1.5.25 2,3,4,4',6-Pentabromodiphenyl ether (BDE-115)

Common Name: 2,3,4,4',6-Pentabromodiphenyl ether

Synonym: PBDE-115, BDE-115, 1,2,3,5-tetrabromo-4-(4-bromophenoxy)benzene

Chemical Name: 2,3,4,4',6-pentabromodiphenyl ether

CAS Registry No: 446254-78-0

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

101.8 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for penta-BDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for penta-BDE, Alcock et al. 1999)

3.02×10^{-5} ; 3.20×10^{-5} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5219/(T/K) + 13.32$, (GC-RT correlation, Wong et al. 2001)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$:

11.52; 11.20 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

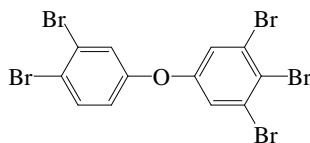
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.26 3,3',4,4',5-Pentabromodiphenyl ether (BDE-126)



Common Name: 3,3',4,4',5-Pentabromodiphenyl ether

Synonym: PBDE-126, BDE-126, 1,2,3-tribromo-5-(3,4-dibromophenoxy)-benzene

Chemical Name: 3,3',4,4',5-pentabromodiphenyl ether

CAS Registry No: 366791-32-4

Molecular Formula: $C_{12}H_5Br_5O$

Molecular Weight: 564.687

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

312.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

6.47×10^{-7} (calculated for pentaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

7.33×10^{-5} – 1.43×10^{-5} (for pentabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.07 (estimated for penta-PBDEs, Alcock et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.64–6.97 (range for penta-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.64–6.97 (quoted range for penta-PBDE, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.97* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -8.41 + 6077/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

12.642, 12.001, 11.441, 10.611 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

12.544, 11.964, 11.423, 10.915 (15 , 25 , 35 , $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.26.1

Reported octanol-air partition coefficients of 3,3',4,4',5-pentabromodiphenyl ether (PBDE 126) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
15	12.642	15	12.574
25	12.001	25	11.992
35	11.441	35	11.449
45	10.611	45	10.939
25	11.97	QRSETP model 5	
log K _{OA} = A + B/(T/K)		15	12.544
A	-8.41	25	11.964
B	6077	35	11.423
enthalpy of phase change		45	10.915
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 116.0$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

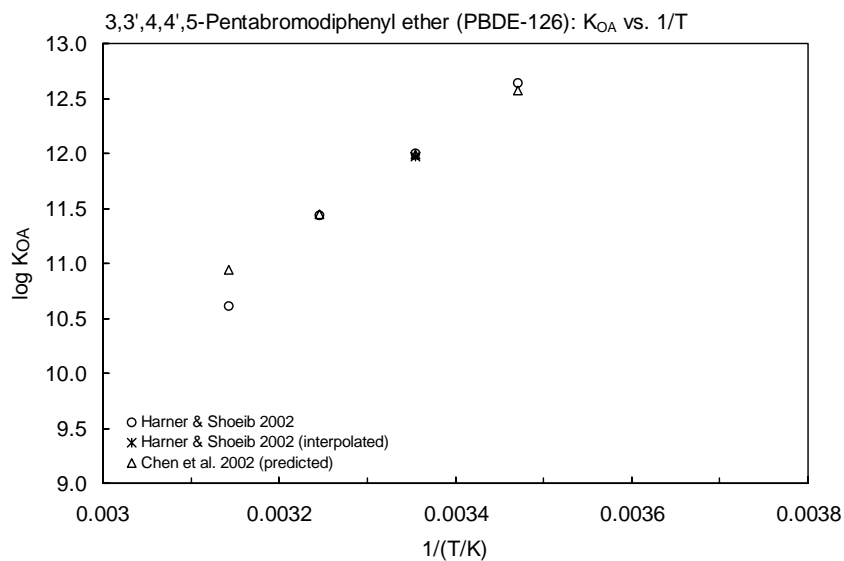
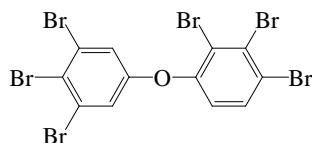


FIGURE 10.1.5.26.1 Logarithm of K_{OA} versus reciprocal temperature for 3,3',4,4',5-pentabromodiphenyl ether (PBDE-126).

10.1.5.27 2,3,3',4,4',5'-Hexabromodiphenyl ether (BDE-138)



Common Name: 2,3,3',4,4',5'-Hexabromodiphenyl ether

Synonym: PBDE-138, BDE-138, 1,2,3-tribromo-4-(2,4,5-tribromophenoxy)-benzene

Chemical Name: 2,3,3',4,4',5'-hexabromodiphenyl ether

CAS Registry No: 182677-30-1

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.584

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

114.06 (Tittlemier & Tomy 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexaBDE, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

9.44×10^{-6} – 4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-BDE, Alcock et al. 1999)

1.51×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -5957/(T/K) + 14.17$, (GC-RT correlation, Tittlemier & Tomy 2001)

1.58×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -6191/(T/K) + 14.97$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

7.91 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

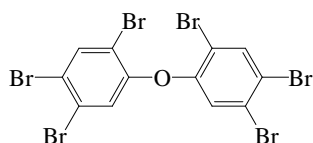
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.28. 2,2',4,4',5,5'-Hexabromodiphenyl ether (BDE-153)



Common Name: 2,2',4,4',5,5'-Hexabromodiphenyl ether

Synonym: PBDE-153, BDE-153, 1,1'-oxybis[2,4,5-tribromophenoxy]-benzene

Chemical Name: 2,2',3,3',5,5'-hexabromodiphenyl ether

CAS Registry No: 68631-49-2

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.583

Melting Point ($^{\circ}C$):

160–163 (Tittlemier et al. 2002)

161.5 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

107.6 (Wong et al. 2001)

110 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

0.045 (calculated at mp $161.5^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexaBDE, Alcock et al. 1999)

8.70×10^{-7} (Solid S_s , generator column-GC/ECD, Tittlemier et al. 2002)

0.0195, 0.0167 (supercooled S_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equation):

9.44×10^{-6} – 4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-BDE, Alcock et al. 1999)

8.43×10^{-6} ; 5.80×10^{-8} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -5620/(T/K) + 13.78$, (GC-RT correlation, Wong et al. 2001)

2.09×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5763/(T/K) + 13.66$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

7.58×10^{-6} , 8.87×10^{-6} (supercooled P_L , selected measured value, final adjusted value, Wania & Dugani 2003)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.067 (calculated- P_L/C_L , Tittlemier et al. 2002)

0.342 (Wania & Dugani 2003)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.86–7.93 (hexabromodiphenyl ethers, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

7.39 (mean value of Watanabe & Tatsukawa, Gustafsson et al. 1999)

7.62 (estimated, Tittlemier et al. 2002)

7.13, 7.08 (selected measured value, final adjusted value, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.82* (generator column-GC/MS, measured range 15–45°C, Harner & Shoeib 2002)

$\log K_{OA} = -5.39 + 5131/(T/K)$, temp range 15–45°C (generator column-GC/MS, Harner & Shoeib 2002)

12.708, 12.127, 11.583, 11.074 (15, 25, 35, 45°C, calculated-QRSETP model 3, Chen et al. 2002)

12.556, 11.977, 11.435, 10.928 (15, 25, 35, 45°C, calculated-QRSETP model 5, Chen et al. 2002)

12.15; 11.78 (calibrated GC-RT correlation; GC-RT correlation, Wania et al. 2002)

11.82, 11.89 (selected measured value, final adjusted value, Wania & Dugani 2003)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 19 \text{ L d}^{-1} \text{ g}^{-1}$ dry wt. in blue mussels (Gustafsson et al. 1999)

$k_2 = 0.086 \text{ d}^{-1}$ in blue mussels (Gustafsson et al. 1999)

$k_2 = 0.051 \text{ d}^{-1}$ with $t_{1/2} = 13.6 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 1110 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Biota: depuration $t_{1/2} = 8.1 \text{ d}$ in blue mussels (Gustafsson et al. 1999);

$t_{1/2} = 13.6 \pm 9 \text{ d}$ in carp (Stapleton et al. 2004a)

depuration $t_{1/2} = 13.6 \text{ d}$ (juvenile carp in 100-d experiment Stapleton et al. 2004b)

TABLE 10.1.5.28.1

Reported octanol-air partition coefficients of 2,2',4,4',5,5'-hexabromodiphenyl ether (PBDE 153) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
$t/^\circ\text{C}$	$\log K_{OA}$	$t/^\circ\text{C}$	$\log K_{OA}$
QRSETP* model 3			
15	12.318	15	12.708
25	11.86	25	12.127
35	11.569	35	11.583
45	10.534	45	11.074
25	11.82	QRSETP model 5	
$\log K_{OA} = A + B/(T/K)$		15	12.556
A	-5.39	25	11.977
B	5131	35	11.435
		45	10.928
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 98.2$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

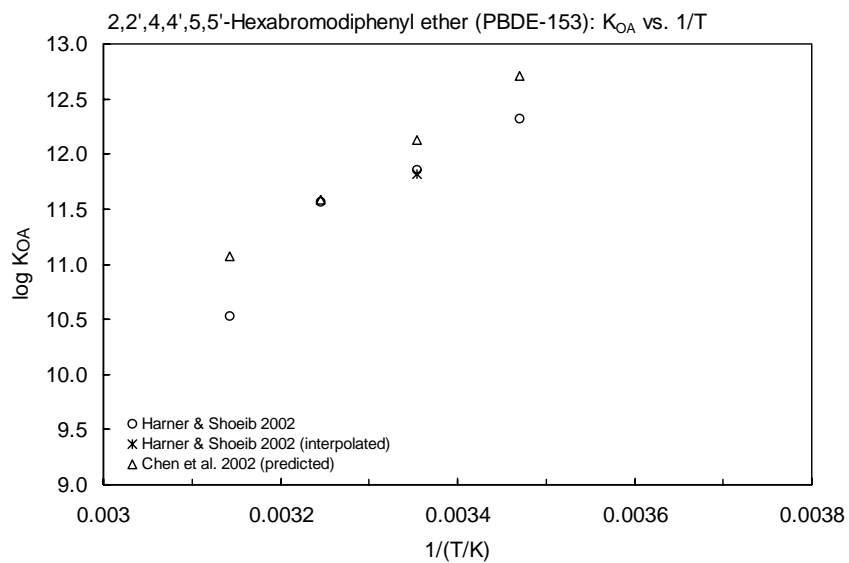
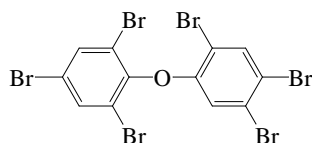


FIGURE 10.1.5.28.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',5,5'-hexabromodiphenyl ether (PBDE-153).

10.1.5.29 2,2',4,4',5,6'-Hexabromodiphenyl ether (BDE-154)



Common Name: 2,2',4,4',5,6'-Hexabromodiphenyl ether

Synonym: PBDE-154, BDE-154, 1,3,5-tribromo-2-(2,4,5-tribromophenoxy)-benzene

Chemical Name: 2,2',4,4',5,6'-hexabromodiphenyl ether

CAS Registry No: 207122-15-4

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.583

Melting Point ($^{\circ}C$):

131–132.5 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

113 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexa-PBDEs, Alcock et al. 1999)

8.70×10^{-7} (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$):

9.44×10^{-6} – 4.22×10^{-6} (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-PBDEs, Alcock et al. 1999)

3.80×10^{-6} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -5900/(T/K) + 14.38$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.24 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

7.39 (estimated, Tittlemier et al. 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section

11.92* (generator column-GC/MS, measured range 15 – $45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -4.62 + 4931/(T/K)$, temp range: 15 – $45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

12.471, 11.890, 11.346, 10.837 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

12.361, 11.782, 11.240, 10.733 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 2.0 \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 35 \text{ d}$ in juvenile carp (Stapleton et al. 2004a)

Half-Lives in the Environment:

Biota: depuration $t_{1/2} = 35 \pm 18 \text{ d}$ in juvenile carp (Stapleton et al. 2004a)

TABLE 10.1.5.29.1

Reported octanol-air partition coefficients of 2,2',4,4',5,6'-hexabromodiphenyl ether (PBDE 154) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K_{OA}	t/°C	log K_{OA}
QRSETP* model 3			
15	12.455	15	12.471
25	11.935	25	11.89
35	11.531	35	11.346
45	10.789	45	10.837
25	11.92	QRSETP model 5	
		15	12.361
		25	11.782
		35	11.24
		45	10.733
log $K_{OA} = A + B/(T/K)$			
A	-4.62		
B	4931		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 94.4$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

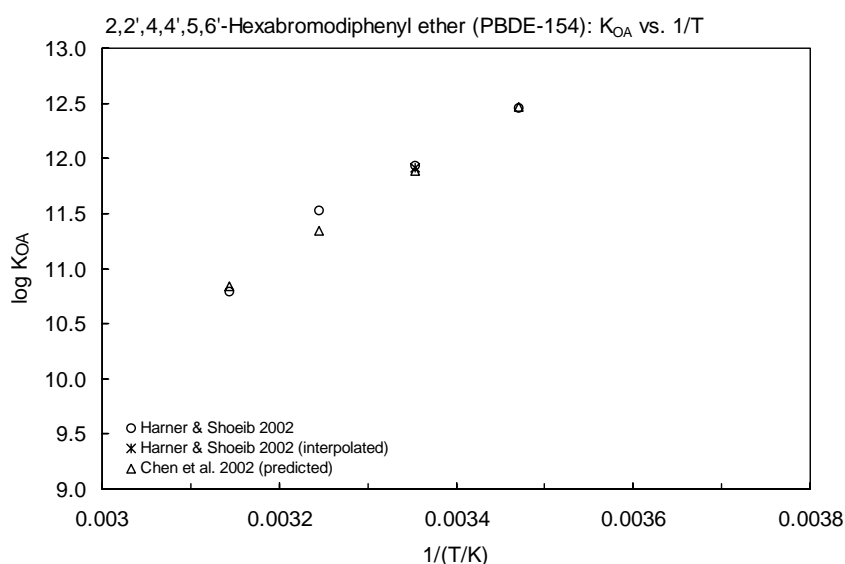
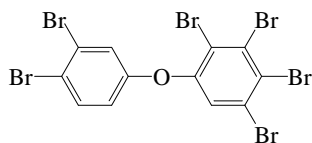


FIGURE 10.1.5.29.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',4,4',5,6'-hexabromodiphenyl ether (PBDE-154).

10.1.5.30 2,3,3',4,4',5-Hexabromodiphenyl ether (BDE-156)



Common Name: 2,3,3',4,4',5-Hexabromodiphenyl ether

Synonym: PBDE-156, BDE-156, 1,2,3,4-tetrabromo-5-(3,4-dibromophenoxy)-benzene

Chemical Name: 2,3,3',4,4',5-hexabromodiphenyl ether

CAS Registry No: 405237-85-6

Molecular Formula: $C_{12}H_4Br_6O$

Molecular Weight: 643.583

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

335.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.08×10^{-6} (calculated for hexa-PBDEs, Alcock et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

$9.44 \times 10^{-6} - 4.22 \times 10^{-6}$ (for hexabromodiphenyl ethers, GC-RT correlation, Watanabe & Tatsukawa 1989)

0.95–0.99 (estimated for hexa-PBDEs, Alcock et al. 1999)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

6.86–7.93 (range for hexa-PBDEs, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

6.86–7.92 (quoted range for hexa-PBDEs, Pijnenburg et al. 1995; Alcock et al. 1999)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.97* (generator column-GC/MS, measured range $15-45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -5.80 + 5298/(T/K)$, temp range: $15-45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

13.211, 12.630, 12.087, 11.577 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

13.150, 12.571, 12.029, 11.522 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 10.1.5.30.1

Reported octanol-air partition coefficients of 2,3,3',4,4',5'-hexabromodiphenyl ether (PBDE 156) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
QRSETP* model 3			
15	-	15	13.211
25	11.976	25	12.63
35	-	35	12.087
45	10.858	45	11.577
25	11.97	QRSETP model 5	
log K _{OA} = A + B/(T/K)		15	13.15
A	-5.80	25	12.571
B	5298	35	12.029
enthalpy of phase change		45	11.522
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 101.0$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

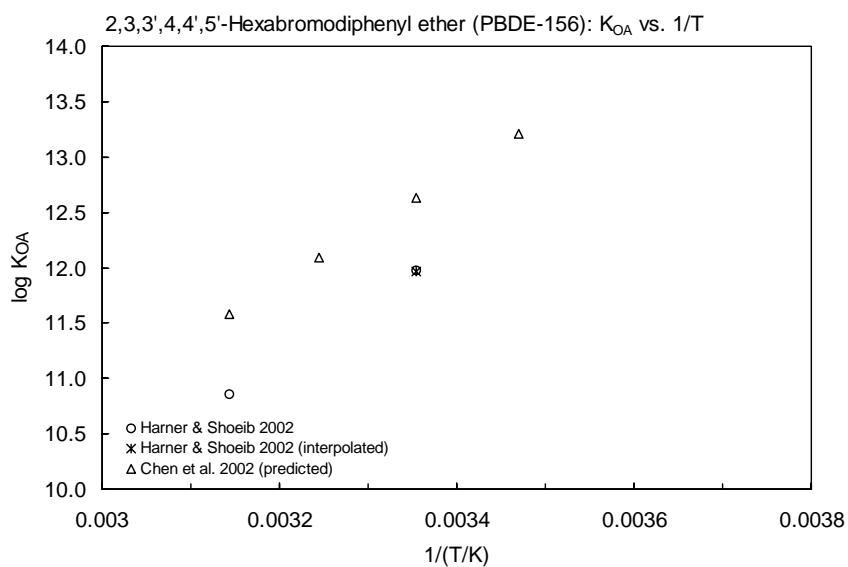
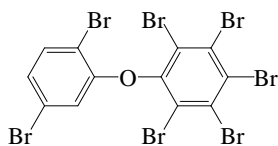


FIGURE 10.1.5.30.1 Logarithm of K_{OA} versus reciprocal temperature for 2,3,3',4,4',5'-hexabromodiphenyl ether (PBDE-156).

10.1.5.31 2,2',3,4,5,5',6-Heptabromodiphenyl ether (BDE-183)



Common Name: 2,2',3,4,5,5',6-Heptabromodiphenyl ether

Synonym: PBDE-183, BDE-183, 1,2,3,5-tetrabromo-4-(2,4,5-trobromophenoxy)-benzene

Chemical Name: 2,2',3,4,5,5',6-heptabromodiphenyl ether

CAS Registry No: 207122-16-5

Molecular Formula: $C_{12}H_3Br_7O$

Molecular Weight: 722.479

Melting Point ($^{\circ}C$):

171–173 (Tittlemier et al. 2002)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

358.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

118 (Tittlemier et al. 2002)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

0.035 (calculated at mp $172^{\circ}C$, Wania & Dugani 2003)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.50×10^{-6} (generator column-GC/ECD, Tittlemier et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and the reported temperature dependence equations):

4.68×10^{-7} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -6185/(T/K) + 14.43$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0074 (calculated- P_L/C_L , Tittlemier et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.14 (quoted, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations.

Additional data at other temperatures designated * are compiled at the end of this section:

11.96* (generator column-GC/MS, measured range $15-45^{\circ}C$, Harner & Shoeib 2002)

$\log K_{OA} = -3.71 + 4672/(T/K)$, temp range: $15-45^{\circ}C$ (generator column-GC/MS, Harner & Shoeib 2002)

13.263, 12.681, 12.138, 11.628 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 3, Chen et al. 2002)

13.206, 12.627, 12.085, 11.577 (15, 25, 35, $45^{\circ}C$, calculated-QRSETP model 5, Chen et al. 2002)

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Air: first-order degradation $t_{1/2} = 1540$ h (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first-order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400$ h (estimated by EPIWIN, Wania & Dugani 2003)

Soil: first order degradation $t_{1/2} = 3600$ h (estimated by EPIWIN, Wania & Dugani 2003)

Biota:

TABLE 10.1.5.31.1

Reported octanol-air partition coefficients of 2,3,3',4,4',5'-hexabromodiphenyl ether (PBDE 183) at various temperatures

Harner & Shoeib 2002		Chen et al. 2002	
generator column-GC/MS		quantitative predictive model	
t/°C	log K _{OA}	t/°C	log K _{OA}
15	-	15	13.263
25	11.964	25	12.681
35	11.477	35	12.138
45	10.978	45	11.628
25	11.96	QRSETP model 5	
		15	13.206
		25	12.627
		35	12.085
		45	11.577
log K _{OA} = A + B/(T/K)			
A	-3.71		
B	4672		
enthalpy of phase change			
$\Delta H_{OA}/(\text{kJ mol}^{-1}) = 89.5$			

note: *QRSETP - quantitative relationships between structures, environmental temperatures and properties.

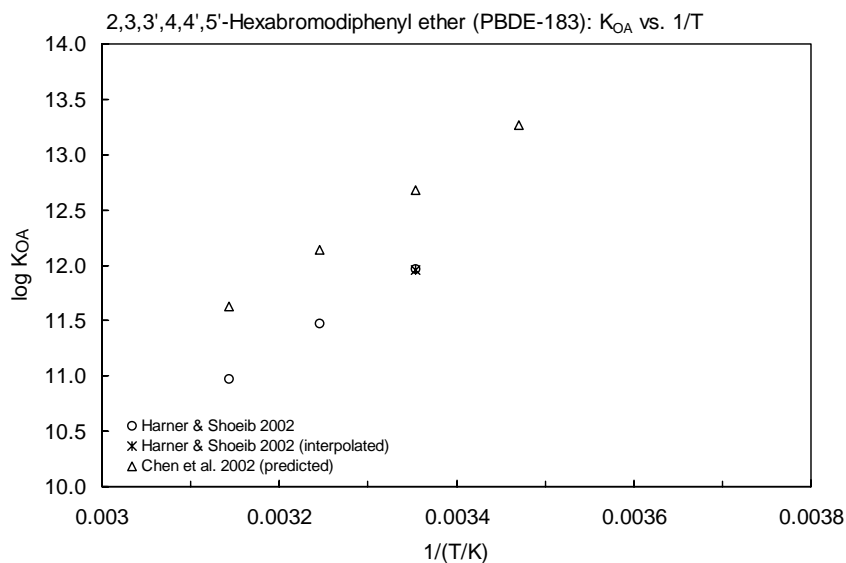
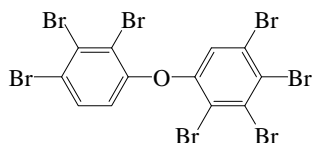


FIGURE 10.1.5.31.1 Logarithm of K_{OA} versus reciprocal temperature for 2,2',3,4,4',5',6-heptabromodiphenyl ether (PBDE-183).

10.1.5.32 2',3,3',4,4',5,6-Heptabromodiphenyl ether (BDE-190)



Common Name: 2',3,3',4,4',5,6-Heptabromodiphenyl ether

Synonym: PBDE-190, BDE-190, pentabromo-(3,4-dibromophenoxy)-benzene

Chemical Name: 2',3,3',4,4',5,6-heptabromodiphenyl ether

CAS Registry No: 189084-68-2

Molecular Formula: $C_{12}H_3Br_7O$

Molecular Weight: 722.479

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

358.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

121.15 (Tittlemier & Tomy 2001)

115.8 (Wong et al. 2001)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

Vapor Pressure (Pa at $25^{\circ}C$ at $25^{\circ}C$ and reported temperature dependence equation):

2.34×10^{-7} (supercooled liquid P_L : GC-RT correlation, Tittlemier & Tomy 2001)

$\log(P_L/Pa) = -6327/(T/K) + 14.60$, (GC-RT correlation, Tittlemier & Tomy 2001)

9.05×10^{-7} ; 5.70×10^{-7} (supercooled liquid P_L : calibrated GC-RT correlation; GC-RT correlation, Wong et al. 2001)

$\log(P_L/Pa) = -6048/(T/K) + 14.24$, (GC-RT correlation, Wong et al. 2001)

2.82×10^{-7} (supercooled liquid P_L : GC-RT correlation, Tittlemier et al. 2002)

$\log(P_L/Pa) = -6552/(T/K) + 15.44$, (Clausius-Clapeyron eq. from GC-RT correlation, Tittlemier et al. 2002)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.36 (estimated, Tittlemier et al. 2002)

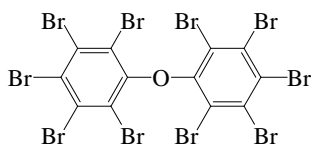
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

10.1.5.33 Decabromodiphenyl ether (BDE-209)

Common Name: Decabromodiphenyl ether

Synonym: PBDE-209, BDE-209, 1,1'-oxybis[2,3,4,5,6-pentabromo]-benzene, bis(pentabromophenyl)-ether, 102(E), 2,2',3,3',4,4',5,5',6,6'-decabromodiphenyl ether, Decabromobiphenyl oxide, decabromophenyl ether

Chemical Name: decabromodiphenyl ether

CAS Registry No: 1163-19-5

Molecular Formula: $C_{12}Br_{10}O$

Molecular Weight: 959.167

Melting Point ($^{\circ}C$):

302.5 (Wania & Dugani 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Molar Volume (cm^3/mol):

428.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4.17×10^{-9} (solid S_s , quoted lit., Wania & Dugani 2003)

Vapor Pressure (Pa at $25^{\circ}C$):

2.95×10^{-9} (supercooled liquid P_L , estimated, Wania & Dugani 2003)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

9.97 (decabromodiphenyl ether, reversed phase-HPLC-RT correlation, Watanabe & Tatsukawa 1989)

9.97 (quoted from Watanabe & Tatsukawa 1990, Pijnenburg et al. 1995)

9.97 (quoted, Wania & Dugani 2003)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{1/2} < 0.25$ h on silica gel, $t_{1/2} = 12$ h on sand, $t_{1/2} = 40$ – 60 h on sediment and $t_{1/2} = 150$ – 200 h in soil; for outdoors under sunlight "discontinuous": $t_{1/2} = 37$ h on sand and 80 h on sediment; for outdoor sunlight "continuous": $t_{1/2}(\text{calc}) = 13$ h on sand and $t_{1/2}(\text{calc}) = 30$ on sediment (Söderström et al. 2004)

Photooxidation:

Hydrolysis:

Biodegradation: anaerobic degradation decreased by 30% within 238 d corresponding to a pseudo-first-order $k = 1 \times 10^{-3} d^{-1}$ by sewage sludge collected from a mesophilic digester (Gerecke et al. 2005)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_2 = 1.4 \times 10^{-2} \text{ d}^{-1}$ with $t_{1/2} = 50 \text{ d}$ in juvenile carp (Stapleton et al. 2004)

Half-Lives in the Environment:

Air: first order degradation $t_{1/2} = 7620 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Surface water: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003)

Ground water:

Sediment: first order degradation $t_{1/2} = 14400 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003); photolysis half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{1/2} = 40\text{--}60 \text{ h}$ on sediment; for outdoors under sunlight "discontinuous": $t_{1/2} = 80 \text{ h}$ on sediment; for outdoor sunlight "continuous": $t_{1/2}(\text{calc}) = 30$ on sediment (Södertröm et al. 2004)

Soil: first order degradation $t_{1/2} = 3600 \text{ h}$ (estimated by EPIWIN, Wania & Dugani 2003); photolysis half-lives on different matrices, indoors under artificial UV-light "continuous": $t_{1/2} = 12 \text{ h}$ on sand, and $150\text{--}200 \text{ h}$ in soil; for outdoors under sunlight "discontinuous": 37 h on sand; for outdoor sunlight "continuous": $t_{1/2}(\text{calc}) = 13 \text{ h}$ on sand (Södertröm et al. 2004)

Biota: depuration $t_{1/2} = 50 \pm 17 \text{ d}$ in juvenile carp (Stapleton et al. 2004)

10.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 10.2.1

Summary of physical properties of ethers and halogenated ethers

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/m³ at 20°C	Molar volume, V _M cm³/mol	
								MW/ρ at 20°C	Le Bas
Aliphatic ethers:									
Dimethyl ether (Methyl ether)	115-10-6	(CH ₃) ₂ O	46.068	−141.5	−24.8	1	0.6689	68.87	60.9
Diethyl ether (Ethyl ether)	60-29-7	(C ₂ H ₅) ₂ O	74.121	−116.2	34.5	1	0.71361	103.87	106.1
Methyl <i>t</i> -butyl ether (MTBE)	1634-04-4	CH ₃ OC(CH ₃) ₃	88.148	−108.6	55	1	0.7404	119.05	127.5
Di- <i>n</i> -propyl ether	111-43-3	(C ₃ H ₇) ₂ O	102.174	−114.8	90.08	1	0.7466	136.85	151.6
Di-isopropyl ether	108-20-3	((CH ₃) ₂ CH) ₂ O	102.174	−85.4	68.4	1	0.73	139.96	151.6
Butyl ethyl ether	628-81-9	(C ₄ H ₉)O(C ₂ H ₅)	102.174	−124	92.3	1	0.7495	136.32	150.5
Di- <i>n</i> -butyl ether	142-96-1	(C ₄ H ₉) ₂ O	130.228	−95.2	140.28	1	0.7684	169.48	196
1,2-Propylene oxide	75-56-9	C ₃ H ₆ O	58.079	−111.9	35	1			69.7
Furan	110-00-9	C ₄ H ₄ O	68.074	−85.61	31.5	1	0.9378	72.59	73.5
2-Methylfuran	534-22-5	C ₅ H ₆ O	82.101	−91.3	64.7	1	0.9132	89.90	95.7
Tetrahydrofuran	109-99-9	C ₄ H ₈ O	72.106	−108.44	65	1	0.8892	81.09	88.3
Tetrahydropyran	142-68-7	C ₅ H ₁₀ O	86.132	−49.1	88	1	0.8814	97.72	107
1,4-Dioxane	123-91-1	C ₄ H ₈ O ₂	88.106	11.85	101.5	1	1.0336	85.24	92
Halogenated ethers:									
Epichlorohydrin	106-89-8	C ₃ H ₅ ClO	92.524	−26	118	1	1.18066	78.37	90.6
Chloromethyl methyl ether	107-30-2	ClCH ₂ -O-CH ₃	80.513	−103.5	59.5	1	1.0703	75.22	81.8
Bis(2-chloromethyl)ether	542-88-1	C ₂ H ₄ Cl ₂ O	114.958	−41.5	106	1			102.7
Bis(2-chloroethyl)ether	111-44-4	(ClC ₂ H ₄) ₂ O	143.012	−51.9	178.5	1	1.2192	117.30	147.9
Bis(2-chloroisopropyl)ether	108-60-1	(ClC ₃ H ₆) ₂ O	171.064	−97	187	1	1.11	154.11	193.4
2-Chloroethyl vinyl ether	110-75-8	ClC ₂ H ₄ -O-C ₂ H ₃	106.551	−70	108	1	1.0475	101.72	119.6
Bis(2-chloroethoxy)methane	111-91-1	(ClC ₂ H ₄) ₂ O ₂ CH ₂	173.037		215	1			180.0
Aromatic ethers:									
Anisole (Methoxybenzene)	100-66-3	(C ₆ H ₅)O(CH ₃)	108.138	−37.13	153.7	1	0.994	108.79	127.3
2-Chloroanisole	766-51-8	C ₇ H ₇ ClO	142.583	−26.8	198.5	1	1.1911	119.71	148.2
3-Chloroanisole	2845-89-8	C ₇ H ₇ ClO	142.583		193.5				148.2
4-Chloroanisole	227881	C ₇ H ₇ ClO	142.583	< −18	197.5	1	1.201	118.72	148.2
2,3-Dichloroanisole	1984-59-4	C ₇ H ₆ Cl ₂ O	177.028	32		0.854			169.1
2,6-Dichloroanisole	1984-65-2	C ₇ H ₆ Cl ₂ O	177.028	10		1			169.1

(Continued)

TABLE 10.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Density, ρ g/m ³ at 20°C	Molar volume, V_M cm ³ /mol	
								MW/ ρ at 20°C	Le Bas
2,3,4-Trichloroanisole	54135-80-7	C ₇ H ₅ Cl ₃ O	211.473	70		0.362			190.0
2,4,6-Trichloroanisole	87-40-1	C ₇ H ₅ Cl ₃ O	211.473	61.5	241	0.438			190.0
2,3,4,5-Tetrachloroanisole	938-86-3	C ₇ H ₄ Cl ₄ O	245.918	88		0.241			210.9
2,3,5,6-Tetrachloroanisole	6936-40-9	C ₇ H ₄ Cl ₄ O	245.918	84		0.264			210.9
Veratrole (1,2-Dimethoxybenzene)	91-16-7	C ₈ H ₁₀ O ₂	138.164	22.5	206	1			158.6
4,5-Dichloroveratrole	2772-46-5	C ₈ H ₈ Cl ₂ O ₂	207.054	83		0.270			200.4
3,4,5-Trichloroveratrole	16766-29-3	C ₈ H ₇ Cl ₃ O ₂	241.499	66		0.396			221.3
Tetrachloroveratrole	944-61-6	C ₈ H ₆ Cl ₄ O ₂	275.944	90		0.230			242.2
Phenetole (Ethoxybenzene)	103-73-1	(C ₆ H ₅)O(C ₂ H ₅)	122.164	-29.43	169.81	1	0.9651	126.58	150.3
Benzyl ethyl ether	539-30-0	C ₆ H ₅ CH ₂ OC ₂ H ₅	136.190		186	1	0.949	143.51	172.5
Styrene oxide	96-09-3	C ₈ H ₈ O	120.149	-35.6	194.1	1	1.0500	114.43	136.1
Diphenyl ether	101-84-8	C ₁₂ H ₁₀ O	170.206	26.87	258	0.959	1.0748	158.36	195.6

* Assuming $\Delta S_{\text{fus}} = 56$ J/mol K.

TABLE 10.2.2

Summary of selected physical-chemical properties of ethers and halogenated ethers at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calculated P/C
	Vapor pressure		Solubility			log K _{OW}	
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)		
Aliphatic ethers:							
Dimethyl ether (Methyl ether)	600000	600000	353000	7662	7662	0.1	13.22*
Diethyl ether (Ethyl ether)	71600	71600	60500	816.2	816.2	0.89	87.72
Methyl <i>t</i> -butyl ether (MTBE)	33500	33500	42000	476.5	476.5	0.94	70.31
Di- <i>n</i> -propyl ether	8334	8334	3306	32.35	32.35	2.03	257.6
Di-isopropyl ether	20000	20000	7900	77.31	77.31	1.52	258.7
Butylethyl ether	8200	8200	6500	63.61	63.61	2.03	128.9
Di- <i>n</i> -butyl ether	850	850	230	1.766	1.776	3.21	481.3
1,2-Propylene oxide	71000	71000	476000	8196	8196	0.03	8.663
Furan	80000	80000	10000	146.9	146.9	1.34	544.6
Tetrahydrofuran	21600	21600	miscible				
Tetrahydropyran	9536	9536	85700	995.0	995.0	0.82	9.584
1,4-Dioxane	5000	5000	miscible			0.27	
Halogenated ethers:							
Epichlorohydrin	2400	2400	65800	771.2	711.2	0.30	3.37
Chloromethyl methyl ether	24900	24900	decompose				
Bis(chloromethyl)ether	4000	4000	22000	191.4	191.4	0.38	20.90
Bis(2-chloroethyl)ether	206	206	10200	71.32	71.32	1.12	2.888
Bis(2-chloroisopropyl)ether	104	104	1700	9.938	9.938	2.58	10.46
2-Chloroethyl vinyl ether	3566	3566	15000	140.8	140.8	1.28	25.33
Bis(2-chloroethoxy)methane	21.6	21.6	81000	468.1	468.1	1.26	0.0461
Aromatic ethers:							
Anisole (Methoxybenzene)	472	472	1600	14.80	14.80	2.11	31.90
2-Chloroanisole			490	3.436	3.436	2.50	
3-Chloroanisole			235	1.648		2.60	
4-Chloroanisole			237	1.662	1.662	2.70	
2,3-Dichloroanisole			86.9	0.4909	0.5748	3.24	
2,6-Dichloroanisole			13.12	0.0741	0.0741	3.14	

(Continued)

TABLE 10.2.2 (Continued)

Compound	Selected properties						Henry's law constant H/(Pa·m³/mol) calculated P/C
	Vapor pressure		Solubility			log K _{OW}	
	P ^S /Pa	P _L /Pa	S/(g/m³)	C ^S /(mol/m³)	C _L /(mol/m³)		
2,3,4-Trichloroanisole			10.8	0.0511	0.1411	4.03	
2,4,6-Trichloroanisole			13.2	0.0624	0.1425	4.02	
2,3,4,5-Tetrachloroanisole			1.35	0.0055	0.0228	4.50	
2,3,5,6-Tetrachloroanisole			1.82	0.0074	0.0280	4.40	
Veratrole (1,2-Dimethoxybenzene)			6690	48.42	48.42	2.18	
4,5-Dichloroveratrole			72	0.2477	1.2879	3.11	
3,4,5-Trichloroveratrole			10.3	0.0426	0.1077	4.01	
Tetrachloroveratrole			1.59	0.0058	0.0250	4.86	
Phenetole (Ethoxybenzene)	204	204	569	4.658	4.658	2.68	43.80
Benzyl ethyl ether	100	100				2.64	
Styrene oxide	40	40	2800	23.30	23.0	1.61	1.716
Diphenyl ether	2.93	3.05	18.7	0.1099	0.1146	4.21	26.67

* Vapor pressure exceeds atmospheric pressure, Henry's law constant H (Pa·m³/mol) = 101325 Pa/C^S mol/m³.

TABLE 10.2.3

Suggested half-life classes of ethers and halogenated ethers in various environmental compartments at 25°C

Compound	Air class	Water* class	Soil class	Sediment class
Aliphatic ethers:				
Dimethyl ether (Methyl ether)	2	5	5	6
Diethyl ether (Ethyl ether)	2	5	5	6
Methyl <i>t</i> -butyl ether (MTBE)	2	5	5	6
Di- <i>n</i> -propyl ether	2	5	5	6
1,2-Propylene oxide	2	4	5	6
Furan	2	4	5	6
Tetrahydrofuran	2	4	5	6
1,4-Dioxane	2	4	5	6
Halogenated ethers:				
Chloromethyl methyl ether	2	5	5	6
Bis(chloromethyl)ether	2	5	5	6
Bis(2-chloroethyl)ether	2	5	5	6
Bis(2-chloroisopropyl)ether	2	5	5	6
2-Chloroethyl vinyl ether	2	5	5	6
Bis(2-chloroethoxy)methane	2	5	5	6
Aromatic ethers:				
Anisole (Methoxybenzene)	2	5	5	6
Styrene oxide	2	4	5	6
Diphenyl ether	2	5	5	6

* Certain ethers will have much shorter half-lives because of hydrolysis with singlet oxygen, and biodegradation; this half-life class is conservatively assigned, see [Chapter 1](#) for a discussion.

where,

	Class	Mean half-life (h)	Range (h)
1		5	< 10
2		17 (~ 1 d)	10–30
3		55 (~ 2 d)	30–100
4		170 (~ 1 week)	100–300
5		550 (~ 3 weeks)	300–1,000
6		1700 (~ 2 months)	1,000–3,000
7		5500 (~ 8 months)	3,000–10,000
8		17000 (~ 2 years)	10,000–30,000
9		55000 (~ 6 years)	> 30,000

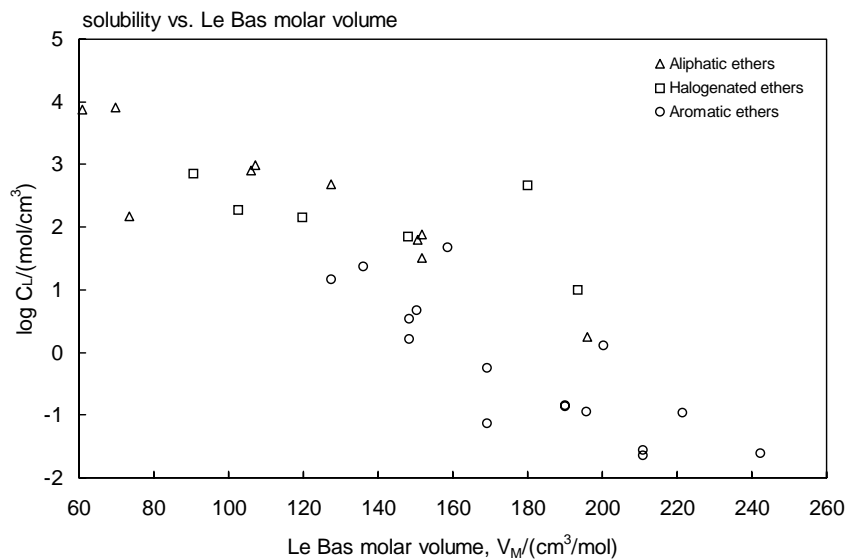


FIGURE 10.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for ethers.

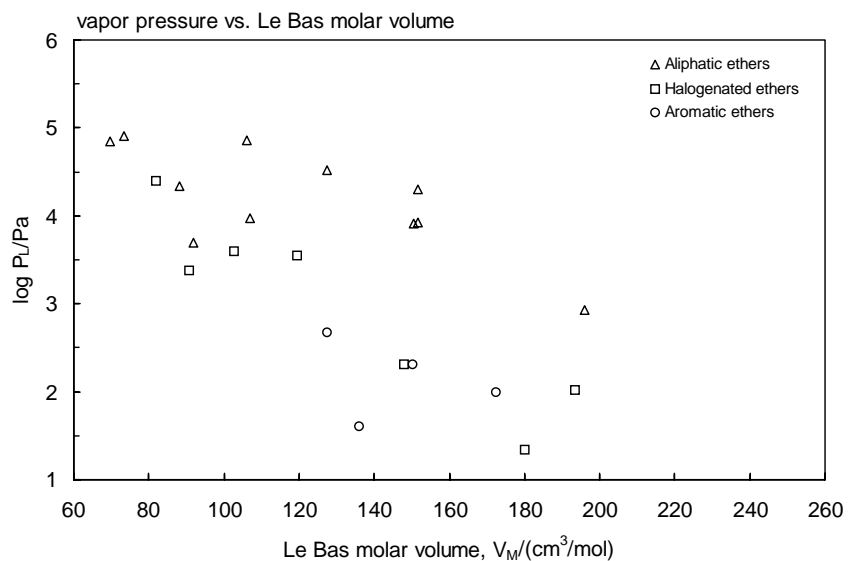


FIGURE 10.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for ethers.

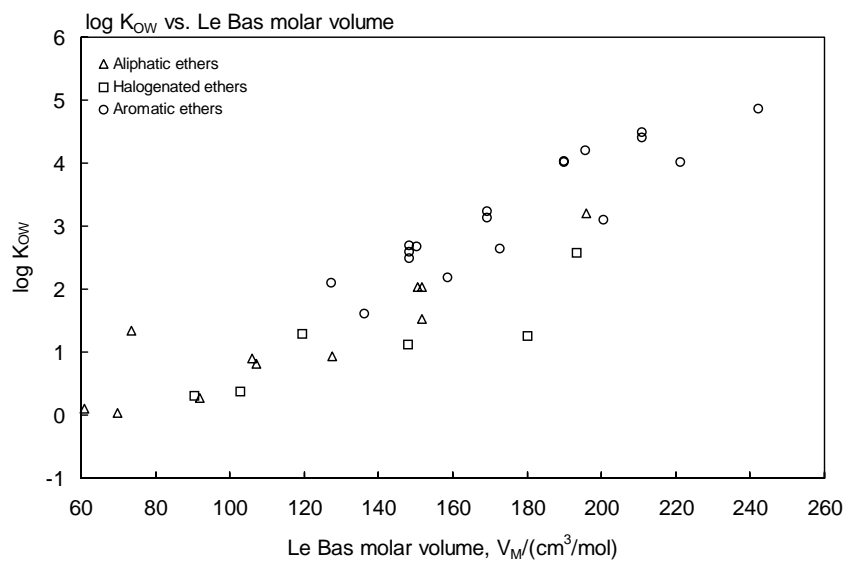


FIGURE 10.2.3 Octanol-water partition coefficient versus Le Bas molar volume for ethers.

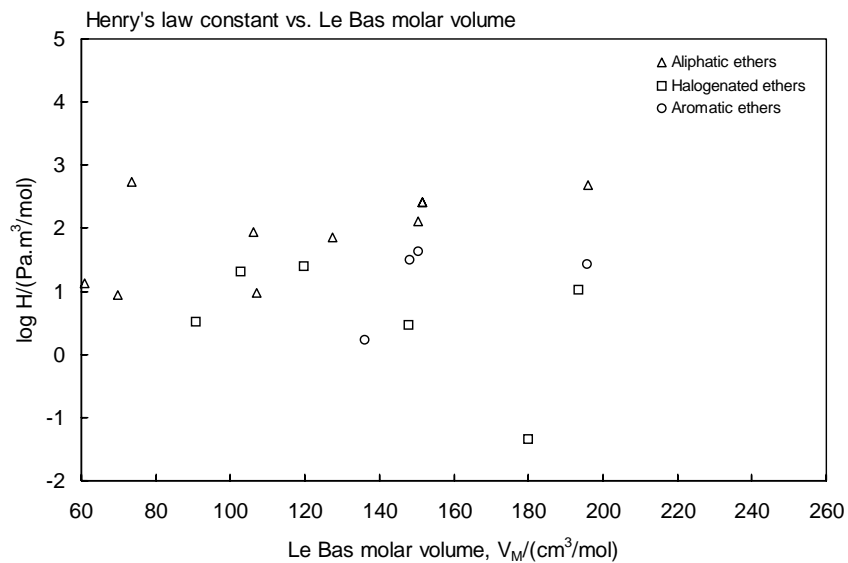


FIGURE 10.2.4 Henry's law constant versus Le Bas molar volume for ethers.

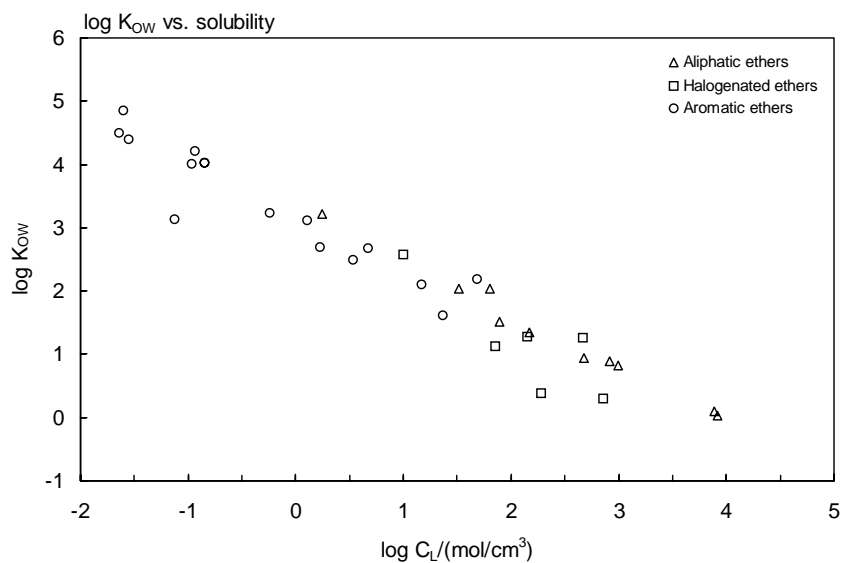


FIGURE 10.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for ethers.

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11 Alcohols

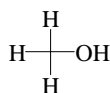
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11.1 LIST OF CHEMICALS AND DATA COMPILATIONS

11.1.1 ALCOHOLS

11.1.1.1 Methanol



Common Name: Methanol

Synonym: methyl alcohol, carbinol, wood alcohol, wood spirit

CAS Registry No: 67-56-1

Molecular Formula: CH₃OH

Molecular Weight: 32.042

Melting Point (°C):

−97.53 (Lide 2003)

Boiling Point (°C):

64.6 (Lide 2003)

Density (g/cm³ at 20°C):

0.7914 (Weast 1982–83)

Molar Volume (cm³/mol):

42.5 (exptl. at normal bp, Lee et al. 1972; quoted, Reid et al. 1977)

40.6 (calculated-density, Rohrschneider 1973)

37.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Dean 1985; Howard 1990)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

16210* (interpolated-regression of tabulated data, temp range −44.0 to 64.7°C, Stull 1947)

16937* (comparative ebulliometry, measured range 15–83.7°C, Ambrose & Sprake 1970)

log (P/Pa) = 7.18411 − 1569.492/(T/K − 34.613); restricted temp range 15–39°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 7.20519 − 1581.933/(T/K − 33.439); temp range 15–83.7°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

16927 (vapor-liquid equilibrium VLE data, Polák & Lu 1972)

log (P/mmHg) = [−0.2185 × 8978.8/(T/K)] + 8.639821; temp range −44 to 224°C (Antoine eq., Weast 1972–73)

16958* (static method, measured range 288.15–337.65 K, Gibbard & Creek 1974)

12260, 21330 (20°C, 30°C, Verschueren 1983)

16960 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 7.24693 − 1806.615/(241.833 + t/°C); temp range 1.72–63.38°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 7.20660 − 1582.698/(239.765 + t/°C); temp range 14–79.63°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

log (P/kPa) = 7.023029 − 1595.671/(240.905 + t/°C), temp range 15–65°C (Antoine eq. derived from exptl data of Gibbard & Creek 1974, Boublik et al. 1984)

16670 (interpolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.89750 − 1474.08/(229.13 + t/°C); temp range −14 to 65°C (Antoine eq., Dean 1985, 1992)

log (P/mmHg) = 7.97328 − 1515.14/(232.85 + t/°C); temp range 64–110°C (Antoine eq., Dean 1985, 1992)

16937 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 7.20519 - 1581.993/(175.47 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P_L/\text{kPa}) = 7.4182 - 1710.2/(-22.25 + T/\text{K})$; temp range 175–273 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.25164 - 1608.39/(-31.07 + T/\text{K})$; temp range 274–337 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.09489 - 1521.23/(-39.18 + T/\text{K})$; temp range 338–487 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.86277 - 1105.884/(-64.272 + T/\text{K})$; temp range 188–228 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.44355 - 1712.316/(-22.61 + T/\text{K})$; temp range 224–290 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.26415 - 1615.59/(-30.437 + T/\text{K})$; temp range 285–345 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.14736 - 1544.804/(-37.235 + T/\text{K})$; temp range 335–376 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.27466 - 1641.542/(-25.789 + T/\text{K})$; temp range 373–458 K (Antoine eq.-VIII, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 45.6171 - 3.2447 \times 10^3/(T/\text{K}) - 13.988 \cdot \log(T/\text{K}) + 6.6365 \times 10^{-3} \cdot (T/\text{K}) - 1.0507 \times 10^{-13} \cdot (T/\text{K})^2$;
 temp range 175–513 K (vapor pressure eq., Yaws 1994)
 35341 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and the reported temperature dependence equations. Additional data at other temperatures designed * are compiled at the end of this section):

0.446 (partial pressure-isoteniscope, Butler et al. 1935)
 0.444 (entrainment method-GC, Burnett 1963)
 0.472 (exptl., Hine & Mookerjee 1975)
 0.367, 0.319 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
 0.45* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.451 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 0.704 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.451 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 0.620 (gas stripping-GC, Altschuh et al. 1999)
 0.506 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 8.969 - 5206.8/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.334 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 3.444 - 2142/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 1.239* (40°C, headspace-GC, measured range 40–65°C, Teja et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

-0.82 (shake flask-CR, Collander 1951)
 -0.66 (shake flask-GC, Hansch & Anderson 1967)
 -0.77 ± 0.02 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
 -0.52 (shake flask-RC, Cornford 1982)
 -0.70 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
 -0.64, -0.63 (quoted, calculated-TSA, Iwase et al. 1985)
 -0.71 (shake flask-GC at pH 7.0, Riebesehl & Tomlinson 1986)
 -0.74 (recommended, Sangster 1989, 1993)
 -0.77 (recommended value, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ as 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

2.98* (20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
 2.84 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

4.45	(alga <i>Chlorella fusca</i> , wet wt. basis, Geyer et al. 1984)
4.45	(alga <i>Chlorella fusca</i> , calculated- K_{OW} , Geyer et al. 1984)
< 1.0	(golden ide, after 3 d, Freitag et al. 1985)
4.46	(algae, after 1 d, Freitag et al. 1985)
2.67	(activated sludge, after 5 d, Freitag et al. 1985)

Sorption Partition Coefficient, log K_{OC} :

-0.23	(calculated-MCI χ , Gerstl & Helling 1987)
0.44	(soil, quoted exptl., Meylan et al. 1992)
-0.36	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
-1.08	(calculated- K_{OW} , Kollig 1993)
0.44	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 5.3$ h and 2.6 d for a model river 1-m deep and an environmental pond (Lyman et al. 1982; selected, Howard 1990).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} ; for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{OH} = (5.7 \pm 0.6) \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ or $9.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

$k_{OH} = (1.06 \pm 0.10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

$k_{OH} = (1.00 \pm 0.10) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

$k_{OH} = 5.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k \sim 0.024 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with O_3 in water at pH 2-5 and 20-23°C (Hoigné & Bader 1983)

$k_{OH} = 0.76 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K in air (Meier et al. 1985; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 6.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 9.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 0.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)

$k_{OH}(\text{exptl}) = 0.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (8.61 \pm 0.47) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240-440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{NO_3} < 6.0 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (flash photolysis-absorption technique (Wallington et al. 1987; selected, Atkinson 1991)

$k(\text{aq.}) = 1.60 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987b)

$k_{OH}(\text{exptl})^* = 8.61 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240-440 (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 8.61 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.60 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 9.32 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (9.0 \pm 0.9) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (1.0 \pm 0.23) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 4.05 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: $t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

estimated $t_{1/2} = 17.8$ d in ambient atmosphere (Howard 1990);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994);

calculated lifetimes of 12 d and 1.0 yr for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water: $t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 1$ d in natural waters (Capel & Larson 1995)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.1.1

Reported vapor pressures of methanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
ln P = A – B/T/K) – C/(T/K)² + D/(T/K)³		(5)					
Stull 1947		Ambrose & Sprake 1970		Gibbard & Creek 1974			
summary of literature data		comparative ebulliometry		static method-manometer			
t/°C	P/Pa	t/°C	P/Pa	T/K	P/kPa	T/K	P/kPa
–44.0	133.3	14.899	9815	288.1506	9.8844	323.1420	55.5900
–25.3	666.6	19.236	12468	288.1508	9.8858	323.1460	55.5996
–16.2	1333	23.323	15519	288.1511	9.8889	323.1490	55.5972
–6.0	2666	27.083	18858	288.1516	9.8867	328.1436	68.8187
5.0	5333	29.911	21769	293.1361	13.0023	328.1442	68.8158
12.1	7999	32.885	25206	293.1443	13.0119	328.1476	68.8450
21.2	13332	35.858	29128	293.1507	13.0109	328.1517	84.5907
34.8	26664	40.637	36493	293.1628	13.0228	333.1417	84.5859
49.9	53329	45.407	45347	298.1478	16.9558	333.1466	84.5940
64.7	101325	48.876	52883	298.1500	16.9562	333.1468	84.5859
		53.315	64036	298.1505	16.9578	333.1471	84.5940
mp/°C	–97.8	56.428	72975	298.1517	16.9584	337.6462	101.2523
		60.814	87345	303.1427	21.8743	337.6456	101.2526
		63.784	98330	303.1464	21.8782	337.6514	101.2742
		64.717	101998	303.1494	21.8823	vapor pressure eq.	
		68.403	117714	303.1503	21.8859		
		71.770	133741	308.1459	27.9763	eq. 5	P/kPa
		75.683	154640	308.1509	27.9844	A	15.6129944
		79.626	178306	308.1521	27.9871	10³B	2.8459280
		83.678	205653	313.1500	35.4685	10⁵C	3.743415457
				313.1504	35.4695	10⁷D	2.188669628
		Antoine eq. for full range		313.1504	35.4714	data also fitted to Cragoe equation, eq. 5 see ref.	
		eq. 3	P/Pa	313.1520	35.4654		
		A	7.20519	318.1475	44.5814		
		B	–1581.93	318.1477	44.5799		
		C	–33.439	318.1483	44.5829		
				318.1506	44.5833		

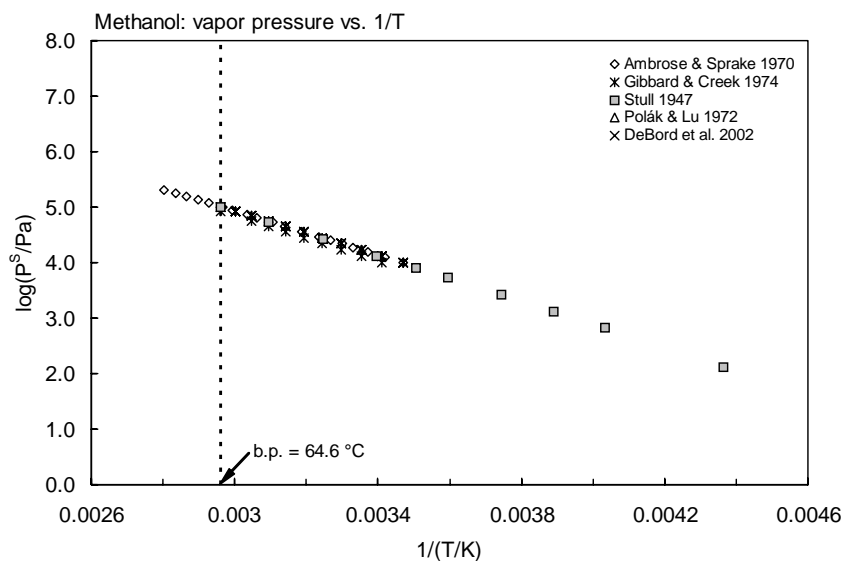


FIGURE 11.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanol.

TABLE 11.1.1.1.2

Reported Henry's law constants and octanol-air partition coefficients of methanol at various temperatures

Henry's law constant		log K_{OA}			
Snider & Dawson 1985		Teja et al. 2001		Gruber et al. 1997	
gas stripping-GC		headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OA}
0	0.0908	40	1.239	20.29	2.98
25	0.4507	50	2.066	30.3	2.76
		60	3.656	40.4	2.56
		65	4.526	50.28	2.40
enthalpy of transfer:					
$\Delta H/(\text{kJ mol}^{-1}) = 41.0$					

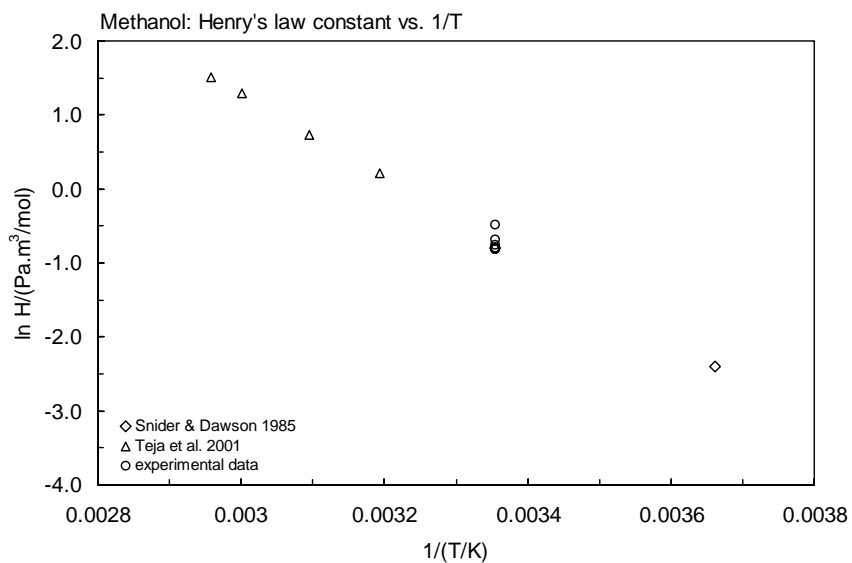


FIGURE 11.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanol.

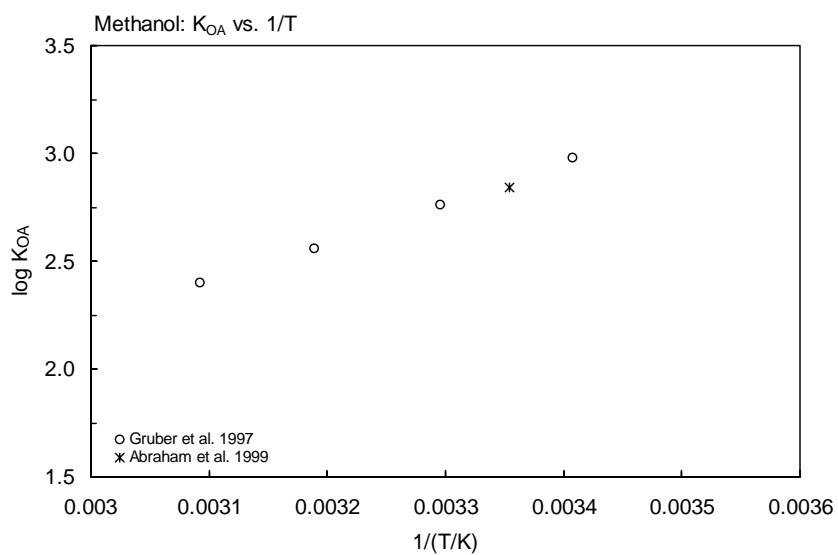


FIGURE 11.1.1.1.3 Logarithm of K_{OA} versus reciprocal temperature for methanol.

11.1.1.2 Ethanol



Common Name: Ethanol

Synonym: ethyl alcohol, methylcarbinol

Chemical Name: ethanol, ethyl alcohol

CAS Registry No: 64-17-5

Molecular Formula: $\text{CH}_3\text{CH}_2\text{OH}$

Molecular Weight: 46.068

Melting Point ($^{\circ}\text{C}$):

-114.14 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

78.29 (Lide 2003)

Density (g/cm^3 at 20°C):

0.78933, 0.78505 (20°C , 25°C , Dreisbach & Martin 1949)

0.7893 (Weast 1982–83)

Molar Volume (cm^3/mol):

58.6 (calculated-density, Rohrschneider 1973)

59.2 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

15.9 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.02 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7314, 7581* (24.4 , 24.8°C , measured range 12.80 – 78.0°C , Kahlbaum 1883)

6906* (22.7°C , static method, measured range 22.7 – 78°C , Smyth & Engel 1929)

7599 (gas saturation/air-bubbling method, Washburn & Handorf 1935)

39345* (vapor-liquid equilibrium VLE data, measured range 35 – 60°C , Scatchard & Raymond 1938)

7538* (interpolated-regression tabulated data, temp range -31.3 to 78.4°C , Stull 1947)

1593, 7869, 29456 (0 , 25 , 50°C , static method, vapor-liquid equilibrium VLE data, Kretschmer et al. 1948)

7869* (static method, measured range 0 – 78.553°C , Kretschmer & Wiebe 1949)

$\log(P/\text{mmHg}) = 8.11576 - 1595.76/(t/^{\circ}\text{C} + 226.5)$; temp range 0 – 78.553°C , Kretschmer & Wiebe 1949)

$\log(P/\text{mmHg}) = 8.24169 - 1652.6/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

7870* (comparative ebulliometry, measured range 19.622 – 93.5°C , Ambrose & Sprake 1970)

$\log(P/\text{Pa}) = 7.16879 - 1552.601/(T/\text{K} - 50.731)$; restricted temp range 19.6 – 43.2°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log(P/\text{Pa}) = 7.24739 - 1599.039/(T/\text{K} - 46.391)$; temp range 19.6 – 93.5°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

7865 (vapor-liquid equilibrium VLE data, Polák & Lu 1972)

$\log(P/\text{mmHg}) = [-0.2185 \times 9673.6/(T/\text{K})] + 8.827392$; temp range -31.3 – 242°C (Antoine eq., Weast 1972–73)

5852, 6665, 9998 (20 , 25 , 30°C , Verschuereen 1983)

8060 (calculated-Antoine eq., Boublik et al. 1984)

- $\log(P/\text{kPa}) = 7.24222 - 1595.811/(226.448 + t/^{\circ}\text{C})$; temp range 19.62–93.48°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 4.11678 - 323.237/(74.916 + t/^{\circ}\text{C})$; temp range 12.8–78.2°C (Antoine eq. from reported exptl. data of Kahlbaum 1883, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 7.31243 - 1630.868/(229.581 + t/^{\circ}\text{C})$; temp range 0–78.55°C (Antoine eq. from reported exptl. data of Kretschmer & Wiebe 1949, Boublik et al. 1984)
 7968 (calculated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 8.32109 - 1718.10/(237.52 + t/^{\circ}\text{C})$; temp range –2 to 100°C (Antoine eq., Dean 1985, 1992)
 7870 (Riddick et al. 1986)
 $\log(P/\text{kPa}) = 7.16879 - 1552.601/(222.419 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 7.15946 - 1547.464/(-51.177 + T/\text{K})$; temp range 320–359 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.23347 - 1591.28/(-47.056 + T/\text{K})$, temp range: 292–367 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.9391 - 2381.5/(T/\text{K})$; temp range 210–271 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.5224 - 2299/(T/\text{K})$; temp range 193–223 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.16386 - 1550.006/(-50.941 + T/\text{K})$; temp range 320–359 K, (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.27664 - 1615.127/(-45.012 + T/\text{K})$; temp range 292–353 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.95131 - 1423.668/(-63.568 + T/\text{K})$; temp range 349–374 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 23.8442 - 2.8642 \times 10^3/(T/\text{K}) - 5.0474 \cdot \log(T/\text{K}) + 3.7448 \times 10^{-11} \cdot (T/\text{K}) + 2.7361 \times 10^{-5} \cdot (T/\text{K})^2$;
 temp range 159–516 K (vapor pressure eq., Yaws 1994)
 17819 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.520 (partial pressure-isoteniscope, Butler et al. 1935)
 0.0118 (partial vapor pressure, concn.-GC, Burnett & Swoboda 1962)
 0.4660 (entrainment method-GC, Burnett 1963)
 0.637 (exptl.-calculated C_w/C_A , Hine & Mookerjee 1975)
 0.495, 0.472 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.527* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.530 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 0.637 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.823 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.70 (correlated-molecular structure, Russell et al. 1992)
 0.542 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 0.593 (solid-phase microextraction SPME-GC, Bartelt 1997)
 0.744 (gas stripping-GC, Altschuh et al. 1999)
 0.568 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{AW} = 10.173 - 5531.6/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.361 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.576 - 2757/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.32 (shake flask-CR, Collander 1951)
 –0.16 (Leo et al. 1969; Hansch & Dunn III 1972)
 –0.30 (shake flask-GC, Dillingham et al. 1973)
 –0.31 ± 0.02 (shake flask-GC, Leo et al. 1975; Hansch & Leo 1979; Hansch & Leo 1985)
 –0.22, –0.20 (calculated-f const., Rekker 1977)
 –0.18 (shake flask-RC, Cornford 1982)

-0.20	(shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
-0.30	(recommended, Sangster 1989, 1993)
-0.25	(thermometric titration, Fujiwara et al. 1991)
-0.29	(calculated-activity coeff. γ from UNIFAC, Dallos et al. 1993)
-0.31, -0.22	(recommended value; value at pH 7.2, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.34*	(20.29°C, from GC determined γ° in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
3.20	(head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

-1.63	(calculated as per Mackay 1982, Schultz et al. 1990)
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Sorption Partition Coefficient, $\log K_{OC}$:

0.09	(calculated- MCI χ , Gerstl & Helling 1987)
0.20	(soil, exptl., Meylan et al. 1992)
-0.14	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
0.20	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 6$ d from water (estimated, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k = 0.01 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 8 \times 10^5$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (1.8 \pm 0.2) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ or $3.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

$k = < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen in aquatic systems at 25°C with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; Mill 1982)

$k_{OH} = 2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at 25°C in the atmosphere with $t_{1/2} = 2.8$ d (Hendry & Kenley 1979)

$k_{OH} = (3.74 \pm 0.37) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978)

$k_{OH} = 1.8 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k_{OH} = (2.62 \pm 0.36) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Ravishankara & Davis 1978)

$k_{OH} = 1.75 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Meier et al. 1985)

$k(aq.) = (0.37 \pm 0.04) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with O_3 in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Zellner & Lorenz 1984; quoted, Carlier et al. 1986)

$k_{OH}(calc) = 3.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(obs.) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}(exptl) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(calc) = 3.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (33.3 \pm 2.3) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{NO_3} < 9.0 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (flash photolysis-absorption technique, Wallington et al. 1987; quoted, Atkinson 1991)

$k_{OH}^* = 3.33 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 3.33 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k(soln) = 3.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}^* = 3.27 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{OH}} = (3.04 \pm 0.25) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{\text{OH}} = (3.46 \pm 0.52) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k(\text{aq.}) = 0.51 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.2, $k = 0.72 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.3, and $k = 0.77 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8.1 for direct reaction with ozone in water at 21°C with $t_{1/2} = 18 \text{ h}$ at pH 7 (Yao & Haag 1991)

$k_{\text{OH}}(\text{calc}) = 5.16 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation screening test data (Heukelekian & Rand 1955; Malaney & Gerhold 1969; selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$k = 0.043\text{--}0.055 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

$t_{1/2} \sim 5.9 \text{ d}$ to 4.0 d estimated in the atmosphere (Graedel 1978; quoted, Howard 1990), based on the reaction with a OH radical concentration of $8 \times 10^5 \text{ molecules/cm}^3$ (Campbell 1976; Lyman et al. 1982; quoted, Howard 1990);

photooxidation $t_{1/2} = 12.2\text{--}122 \text{ h}$, based on measured rate constant for the reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);

calculated lifetimes of 3.5 d and 26 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water: photooxidation $t_{1/2} = 334 \text{ d}$ –36.6 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; selected, Howard et al. 1991); measured rate constants of $0.51 \text{ M}^{-1} \text{ s}^{-1}$, $0.72 \text{ M}^{-1} \text{ s}^{-1}$, $0.77 \text{ M}^{-1} \text{ s}^{-1}$, at pH 7.2, 7.3, 8.1, respectively, for direct reaction with ozone in water at 21°C , with $t_{1/2} = 18 \text{ h}$ at pH 7 (Yao & Haag 1991).

Groundwater: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

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TABLE 11.1.1.2.1

Reported vapor pressures of ethanol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^\circ\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^\circ\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log(T/K) \quad (4)$$

Kahlbaum 1883		Scatchard & Raymond 1938		Kretschmer & Wiebe 1949		Ambrose & Sprake 1970	
Ber. 16, 2476 (1883)		vapor-liquid equilibrium		static method, VLE data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.80	2733	35	13703	0.0	1593	19.622	5726
17.4	4114	40	17877	25.0	7869	23.633	7269
21.0	5509	45	23033	34.988	13736	25.722	8205
24.4	7314	50	29488	44.994	23058	28.157	9430
24.8	7581	55	37312	50.0	29456	33.334	12566

(Continued)

TABLE 11.1.1.2.2
Reported Henry’s law constants and octanol-water partition coefficients of ethanol at various temperatures

Henry’s law constant		log K _{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det’d activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
0	0.0688	20.29	3.34
25	0.5274	30.3	3.10
		40.4	2.87
		50.28	2.69

enthalpy of transfer:
 $\Delta H/(\text{kJ mol}^{-1}) = 54.392$

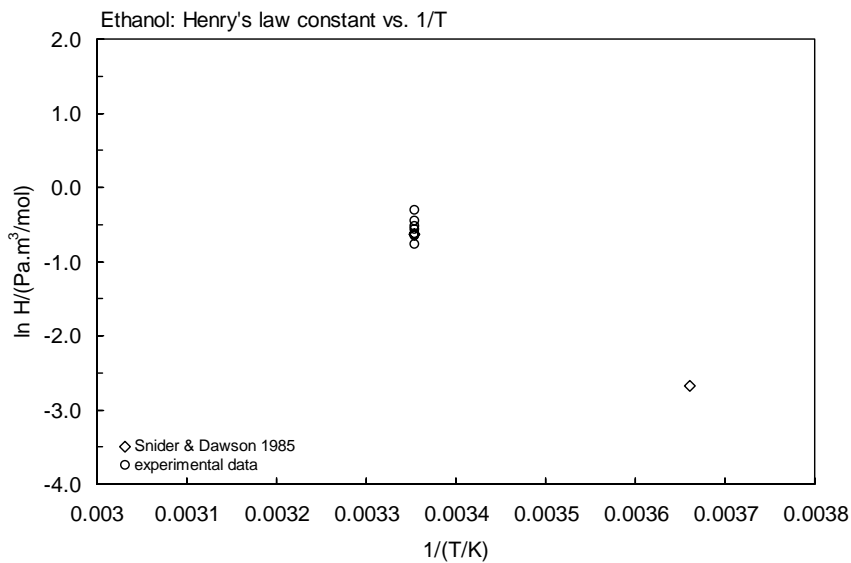


FIGURE 11.1.1.2.2 Logarithm of Henry’s law constant versus reciprocal temperature for ethanol.

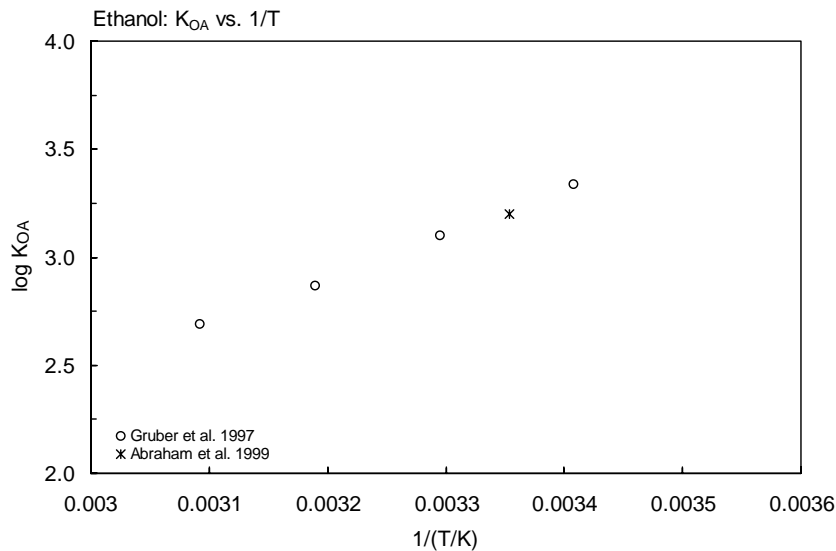
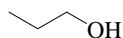


FIGURE 11.1.1.2.3 Logarithm of K_{OA} versus reciprocal temperature for ethanol.

11.1.1.3 Propanol (*n*-Propyl alcohol)

Common Name: Propanol

Synonym: propyl alcohol, 1-propanol, *n*-propyl alcohol

Chemical Name: propanol, propyl alcohol, *n*-propyl alcohol

CAS Registry No: 71-23-8

Molecular Formula: C₃H₈O, CH₃CH₂CH₂OH

Molecular Weight: 60.095

Melting Point (°C):

−124.39 (Lide 2003)

Boiling Point (°C):

97.2 (Lide 2003)

Density (g/cm³ at 20°C):

0.8035 (Weast 1982–83)

0.8037 (Dean 1985)

Molar Volume (cm³/mol):

75.1 (calculated-density, Rohrschneider 1973)

81.4 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK:

19.4 (pK_s, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.372 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

> 3.1 × 10⁶ (Booth & Everson 1948)

miscible (Dean 1985; Riddick et al. 1986, Yaws et al. 1990))

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2844 (saturated vapor density-gas saturation, Puck & Wise 1946)

2594* (interpolated-regression of tabulated data, temp range −15 to 97.8°C, Stull 1947)

10990* (48.14°C, measured range 48.14–97.1°C, Brown & Smith 1959)

2720* (ebulliometry-differential thermal analysis, measured range 19.3–97.3°C, Kemme & Kreps 1969)

log (P/mmHg) = 8.18894 − 1690.864/(221.346 + t/°C); temp range 19.3–97.3°C, or pressure range 14.7–758.5 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

2798* (comparative ebulliometry, measured range 60.2–104.5°C, Ambrose & Sprake 1970)

log (P/Pa) = 6.74390 − 1365.579/(T/K − 82.093); restricted temp range 60.2–81.2°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 6.87613 − 1441.705/(T/K − 74.291); temp range 60.2–104.5°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/mmHg) = [−0.2185 × 10421.1/(T/K)] + 8.937293; temp range −15 to 250°C (Antoine eq., Weast 1972–73)

2744 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.97878 − 1497.734/(204.094 + t/°C); temp range 48.14–94.36°C (Antoine eq. from reported exptl. data of Brown & Smith 1959, Boublik et al. 1984)

log (P/kPa) = 6.87065 − 1438.587/(198.552 + t/°C); temp range 60.2–104.6°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

2780 (interpolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.84767 − 1499.21/(204.64 + t/°C); temp range 2–120°C (Antoine eq., Dean 1985, 1992)

2798 (Riddick et al. 1986)

log (P/kPa) = 6.87613 − 1441.705/(198.859 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

- $\log (P_L/\text{kPa}) = 6.86874 - 1437.906/(-74.621 + T/\text{K})$; temp range 333–378 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.74195 - 1364.911/(-82.114 + T/\text{K})$; temp range 356–378 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.7592 - 2506/(T/\text{K})$; temp range 200–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.74403 - 1366.08/(-81.994 + T/\text{K})$; temp range 356–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.87377 - 1440.743/(-74.344 + T/\text{K})$; temp range 333–376 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.58415 - 1273.365/(-92.178 + T/\text{K})$; temp range 369–407 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 31.5155 - 3.457 \times 10^3/(T/\text{K}) - 7.5235 \cdot \log (T/\text{K}) - 4.287 \times 10^{-11} \cdot (T/\text{K}) + 1.3029 \times 10^{-7} \cdot (T/\text{K})^2$;
 temp range 124–537 K (vapor pressure eq., Yaws 1994)
 6939 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)
 9470 (45.43°C, vapor-liquid equilibrium VLE data, measured range 45.43–58.9°C, Pasanen et al. 2004)
 5876 (37.02°C, ebulliometric method, measured range 310.17–356.7 K, Lubomska & Malanowski 2004)
 $\log (P/\text{kPa}) = 7.219284 - 1629.492/[(T/\text{K}) - 57.556]$; temp range 310.17–356.7 K (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.694 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 0.620 (entrainment method-GC, Burnett 1963)
 0.683 (exptl., Hine & Mookerjee 1975)
 0.699; 0.710 (calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
 0.751* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.683 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 0.925 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.683, 0.942 (quoted, correlated-molecular structure, Russell et al. 1992)
 0.715 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 1.034 (solid-phase microextraction SPME-GC, Bartelt 1997)
 0.372 (wetted-wall column-GC, Altschuh et al. 1999)
 0.802 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 11.830 - 5923.2/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.490 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 6.955 - 3123/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.34 (shake flask-GC, Hansch & Anderson 1967)
 0.30 (shake flask-GC, Dillingham et al. 1973)
 0.25 \pm 0.01 (shake flask-GC, Leo et al. 1975)
 0.29 (Hansch & Leo 1979)
 0.32 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 0.25 (recommended, Sangster 1989)
 0.25 (recommended value, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

- 3.85* (20.29°C, from GC determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
 3.20 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.069 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

0.37	(calculated-MCI χ , Gerstl & Helling 1987)
0.48	(soil, quoted exptl., Meylan et al. 1992)
0.12	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
0.48	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated * data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (2.3 \pm 0.2) \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 2 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 2.8$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = (5.33 \pm 0.53) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

$k = (0.37 \pm 0.04) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{exptl}) = 5.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 5.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (5.34 \pm 0.29) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{OH} = 5.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 4.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 5.34 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (5.64 \pm 0.48) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (5.50 \pm 0.44) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at 298 ± 2 K (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 6.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $71.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water:

Groundwater:

Sediment:

Soil:

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TABLE 11.1.1.3.1
Reported vapor pressures of propanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Brown & Smith 1959		Kemme & Kreps 1969		Ambrose & Sprake 1970	
summary of literature data				differential thermal analysis		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
ebulliometry							
−15.0	133.1	48.14	10990	19.3	1960	60.168	20438
5.0	666.6	48.16	10996	19.8	1987	65.599	26579
14.7	1333	48.18	11018	24.5	2720	70.255	33024
25.3	2666	54.52	15405	30.3	3920	74.507	40001
36.4	5333	61.51	21851	30.3	3933	78.022	46676
43.5	7999	65.80	26867	35.2	5293	81.174	53435
52.8	13332	70.09	32831	41.3	7519	83.931	59974
66.8	26664	74.56	40177	48.1	10839	86.490	66638
82.0	53329	81.11	53379	55.4	16052	88.856	73334
97.8	101325	97.08	101358	65.7	26584	91.026	79952
mp/°C	−127	97.09	101331	74.6	39997	93.143	86877
		97.10	101393	86.6	66461	94.955	93192
		86.0	65456	97.3	101125	96.837	100132
		91.13	80472			97.595	103031
		94.36	91342	Antoine eq.		98.513	106666
				eq. 2	P/mmHg	100.155	113408
		A	8.18894	101.666	119903		
		B	1690.864	103.166	126648		
		C	221.346	104.515	133259		
				$\Delta H_v/(\text{kJ mol}^{-1})$			
				at bp	56.066		

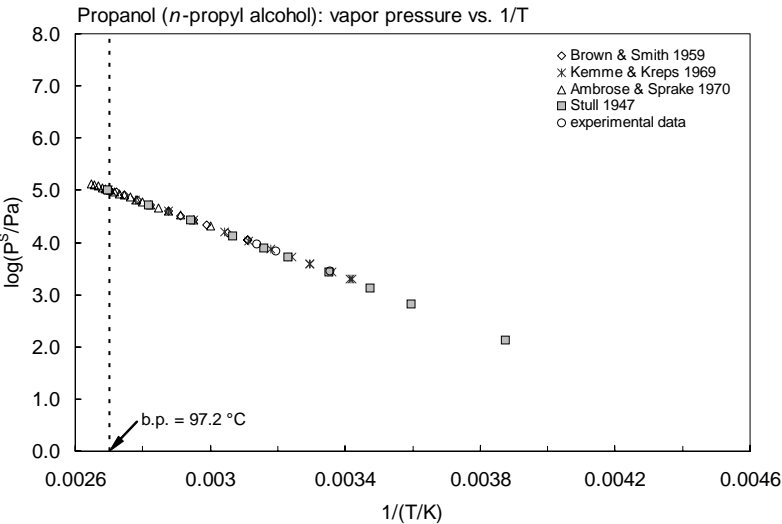


FIGURE 11.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propanol.

TABLE 11.1.1.3.2

Reported Henry's law constants and octanol-air partition coefficients of propanol at various temperatures

Henry's law constant		log K _{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
0	0.0757	20.29	3.85
25	0.7512	30.3	3.56
		40.4	3.33
		50.28	3.11
enthalpy of transfer: $\Delta H/(\text{kJ mol}^{-1}) = 58.576$			

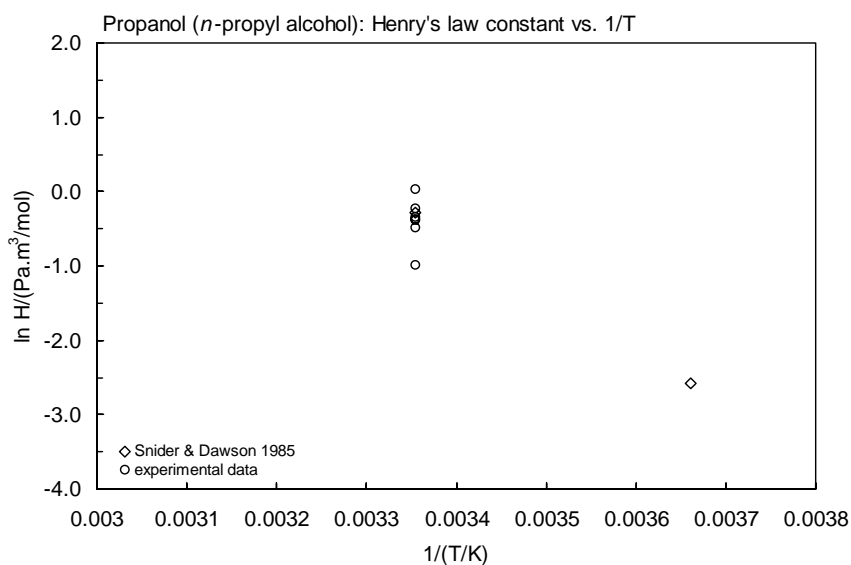
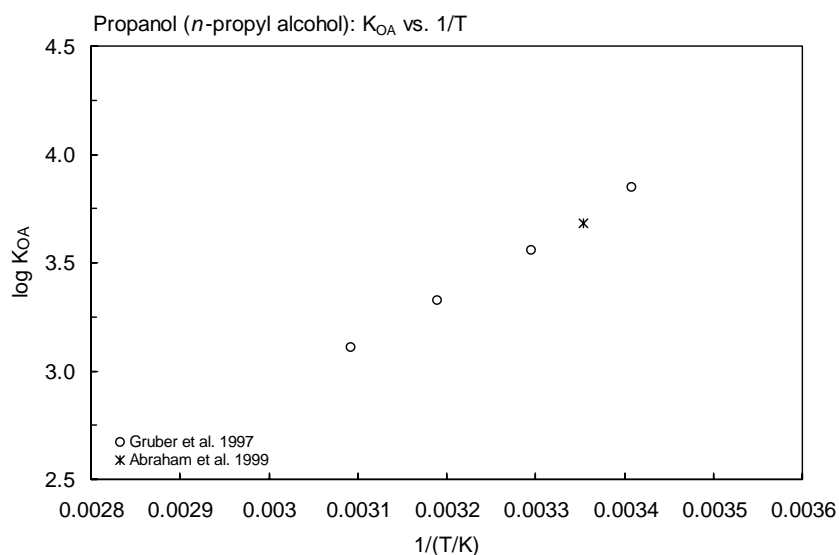


FIGURE 11.1.1.3.2 Logarithm of Henry's law constant versus reciprocal temperature for propanol.

FIGURE 11.1.1.3.3 Logarithm of K_{OA} versus reciprocal temperature for propanol.

11.1.1.4 Isopropanol (*i*-Propyl alcohol)

Common Name: Isopropanol

Synonym: isopropyl alcohol, 2-propanol, *i*-propyl alcohol, dimethylcarbinol, *sec*-propylalcohol, perspirit, petrohol, avantine, IPA

Chemical Name: isopropanol, isopropyl alcohol, *i*-propyl alcohol

CAS Registry No: 67-63-0

Molecular Formula: C_3H_8O , $CH_3(CH_3)CHOH$

Molecular Weight: 60.095

Melting Point ($^{\circ}C$):

−87.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

82.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7812 ($25^{\circ}C$, Butler et al. 1935)

0.7855 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

76.8 (calculated-density, Rohrschneider 1973)

81.4 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

17.1 (Serjeant & Dempsey 1979; Howard 1990)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.406 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

$> 3.1 \times 10^6$ (Booth & Everson 1948)

miscible (Dean 1985; Riddick et al. 1986; Howard 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5866* (static method-isoteniscope, measured 0 – $90^{\circ}C$, Parks & Barton 1928)

5700* (interpolated-regression of tabulated data, temp range -26.1 to $82.5^{\circ}C$, Stull 1947)

5775* (comparative ebulliometry, measured range 52.323 – $89.261^{\circ}C$, Ambrose & Sprake 1970)

$\log(P/Pa) = 6.73896 - 1290.345/(T/K - 82.778)$; restricted temp range 52.3 – $71.1^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log(P/Pa) = 6.86618 - 1360.131/(T/K - 75.558)$; temp range 52.3 – $89.3^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log(P/mmHg) = [-0.2185 \times 10063.5/(T/K)] + 7.805751$; temp range -91 to $160^{\circ}C$ (Antoine eq., Weast 1972–73) 4266, 7588 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

5070; 5700 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.86634 - 1360.183/(197.593 + t/^{\circ}C)$; temp range 52.3 – $89.26^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

$\log(P/kPa) = 6.358 - 1082.462/(166.482 + t/^{\circ}C)$; temp range 81.61 – $147.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6021 (calculated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 8.11778 - 1580.92/(219.61 + t/^{\circ}C)$; temp range 0 – $101^{\circ}C$ (Antoine eq., Dean 1985, 1992)

5775 (Riddick et al. 1986)

$\log(P/kPa) = 6.86618 - 1360.131/(126.36 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 6.86087 - 1357.514/(-75.786 + T/\text{K})$; temp range 325–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.72348 - 1282.26/(-83.591 + T/\text{K})$; temp range 347–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.681 - 2626/(T/\text{K})$; temp range 195–228 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.73782 - 1290.039/(-82.771 + T/\text{K})$; temp range 347–363 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.86451 - 1359.473/(-75.592 + T/\text{K})$; temp range 325–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.61939 - 1225.439/(-89.774 + T/\text{K})$; temp range 350–383 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 38.2363 - 3.5513 \times 10^3/(T/\text{K}) - 10.031 \cdot \log(T/\text{K}) - 3.474 \times 10^{-10} \cdot (T/\text{K}) + 1.7367 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 185–508 K (vapor pressure eq., Yaws 1994)
 13806 (40°C, vapor-liquid equilibrium VLE data, DeBord et al. 2002)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.814 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 0.820 (exptl., Hine & Mookerjee 1975)
 1.159, 0.710 (calculated-group contribution, calculated-bond contribution; Hine & Mookerjee 1975)
 0.80* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 1.131 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 3.16* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln (1/K_{AW}) = -10.6 + 5413/(T/\text{K})$; temp range 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
 0.820, 0.715 (quoted, correlated-molecular structure, Russell et al. 1992)
 1.091 (gas stripping-GC, Altschuh et al. 1999)
 5.55 (EPICS-GC, Ayuttaya et al. 2001)
 0.521 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.576 - 2757/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 2.186 – 0.666 (27°C, equilibrium headspace-GC, solute concn 12.31–125.08 mg/L, measured range 300–315 K, Cheng et al. 2003)
 2.186* (27°C, equilibrium headspace-GC, measured range 27–42°C, Cheng et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.14 (Leo et al. 1969; Hansch & Dunn III 1972)
 0.05 (shake flask-GC, Dillingham et al. 1973)
 0.05 (Hansch & Leo 1985)
 0.14 (HPLC- k' correlation, Funasaki et al. 1986)
 0.55 (UNIFAC activity coefficient, Banerjee & Howard 1988)
 0.05 (recommended, Sangster 1989, 1993)
 0.05 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.54* (20.29°C, from GC determined γ^∞ in octanol, measured range 20.29–50.28°C, Gruber et al. 1997)
 3.38 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: the estimated $t_{1/2} \sim 3.6$ d for evaporation from water 1 m deep with 1 m/s current and 3 m/s wind (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 197$ d to 22 yr in water, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 4.1 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 1.3$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = (5.48 \pm 0.55) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(296 \pm 2) \text{ K}$ (Overend & Paraskevopoulos 1978; quoted, Atkinson 1985)

$k_{OH} = 4.3 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k = (1.9 \pm 0.2) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2–6 and 20–23°C (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 7.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 6.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{exptl}) = 6.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{OH}(\text{calc}) = 6.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (5.81 \pm 0.34) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{NO_3} < 2.3 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (flash photolysis-absorption technique, Wallington et al. 1987; quoted, Atkinson 1991)

$k(\text{aq.}) = 3.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987b)

$k_{OH}(\text{exptl})^* = 5.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH} = 5.81 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 3.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH}^* = 5.21 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{OH} = (5.69 \pm 1.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (5.78 \pm 0.753) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 2.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

$k = 52.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}$ (aq. aerobic) = 24–168 h, based on unacclimated aerobic aqueous screening test data (Gellman & Heukelekian 1955; Heukelekian & Rand 1955; Price et al. 1974; Takemoto et al. 1981; Wagner 1976; selected, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 96–672 h, based on estimated aerobic aqueous biodegradation half-life and unacclimated anaerobic aqueous screening test data (Hou et al. 1983; Sonoda & Seiko 1968; Speece 1983; selected, Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 6.2\text{--}72$ h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985, 1987; quoted, Howard 1990; selected, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 197$ d to 22 yr, based on measured rate constant for the reaction with hydroxyl radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2} = 26$ –168 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ –336 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24$ –168 h, based on estimated unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.4.1

Reported vapor pressures of isopropanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)			
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)			
$\log P = A - B/(C + T/K)$	(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)					
Parks & Barton 1928	Stull 1947	Ambrose & Sprake 1970				
static method/isoteniscope	summary of literature data	comparative ebulliometry				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	
0	1187	−26.1	133.1	52.323	26540	
5	1613	−7.00	666.6	56.779	33044	
10	2266	2.40	1333	60.798	40017	
15	3173	12.7	2666	64.091	46612	
20	4320	23.8	5333	67.087	53371	
25	5866	30.5	7999	69.704	59931	
30	7879	39.5	13332	72.131	66601	
35	10519	53.0	26664	74.372	73286	
40	14079	67.8	53329	76.454	79997	
45	18239	82.5	101325	78.431	86822	
50	23571			80.160	93175	
55	30318	mp/°C	−85.8	81.931	100078	
60	38464			82.958	104266	
65	48409			85.090	113416	
70	60635			86.550	120046	
75	74847			87.992	126573	
80	92232			89.261	133218	
85	112737					
90	136082					
$\Delta H_v/(\text{kJ mol}^{-1}) =$						
at 25°C	44.43					
at bp	40.166					

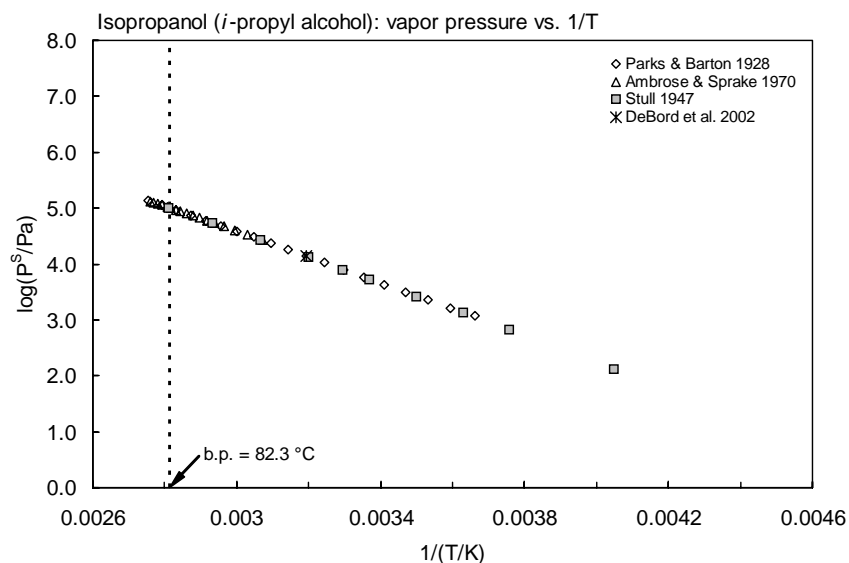


FIGURE 11.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for isopropanol.

TABLE 11.1.1.4.2

Reported Henry's law constants and octanol-air partition coefficients of isopropanol at various temperatures

Henry's law constant				log K_{OA}			
Snider & Dawson 1985		Kolb et al. 1992		Cheng et al. 2003		Gruber et al. 1997	
gas stripping-GC		equilibrium headspace-GC		equilibrium headspace-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	log K_{OA}
0	0.0811	40	3.16	27	2.186	20.29	3.54
25	0.800	60	9.68	32	2.51	30.3	3.27
		70	15.94	37	3.35	40.4	3.04
		80	25.09	42	4.24	50.28	2.85
enthalpy of transfer:							
$\Delta H/(\text{kJ mol}^{-1}) = 58.576$							
		$\ln (1/K_{AW}) = A - B/(T/K)$					
		$1/K_{AW}$					
		A -10.6					
		B -5413					

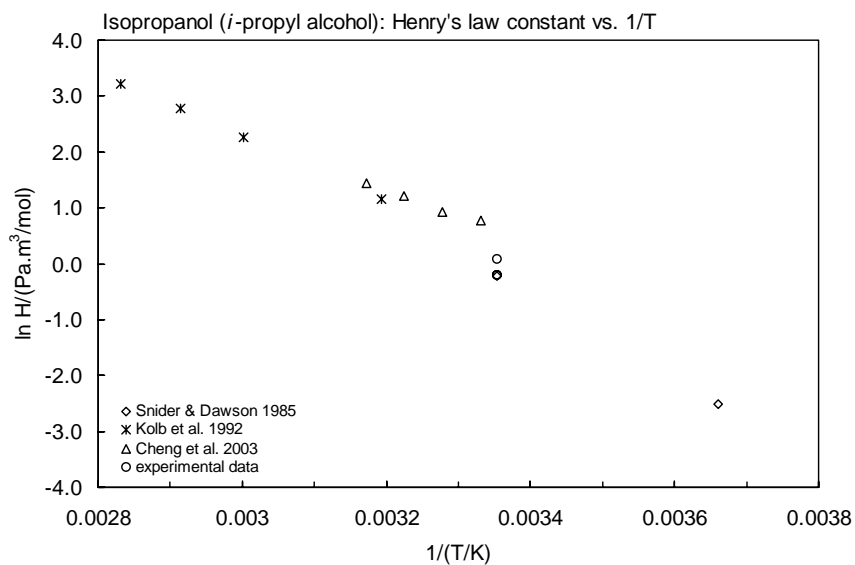


FIGURE 11.1.1.4.2 Logarithm of Henry's law constant versus reciprocal temperature for isopropanol.

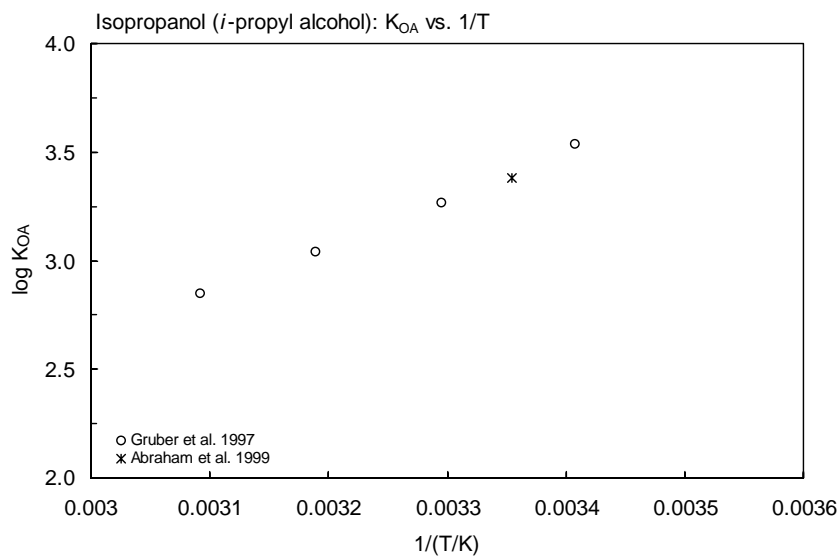
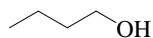


FIGURE 11.1.1.4.3 Logarithm of K_{OA} versus reciprocal temperature for isopropanol.

11.1.1.5 *n*-Butanol (*n*-Butyl alcohol)Common Name: *n*-ButanolSynonym: 1-butanol, *n*-butyl alcohol, *n*-propylcarbinolChemical Name: *n*-butyl alcohol, 1-butanol

CAS Registry No: 71-36-3

Molecular Formula: C₄H₁₀O, CH₃CH₂CH₂CH₂OH

Molecular Weight: 74.121

Melting Point (°C):

-88.6 (Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point (°C):

117.73 (Lide 2003)

Density (g/cm³ at 20°C):

0.80593 (25°C, Butler et al. 1935)

0.80980 (Weast 1982–83)

0.80956, 0.80575 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

91.7 (calculated-density, Rohrschneider 1973)

103.6 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a:

20.89 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.37 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

68120, 79000*	(18, 20°C, shake flask-turbidity, Fühner 1924)
73500*	(volumetric method, Hill & Malisoff 1926)
64000*	(20°C, synthetic method, Jones 1929)
70800*	(30°C, vapor liquid equilibrium, measured range 0–105°C, Mueller et al. 1931)
74500	(gravimetric method, Stockhart & Hull 1931)
73180	(24.85°C, shake flask-interferometer, Butler et al. 1933)
73100	(shake flask-cloud point, Butler et al. 1933)
70000	(26°C, synthetic method, Othmer et al. 1945)
73320	(shake flask-residue volume, Booth & Everson 1948)
74100	(shake flask-interferometry, Hansen et al. 1949)
73000	(shake flask-interferometry, quoted from Butler et al. 1933, Donahue & Bartell 1952)
75850	(estimated, McGowan 1954)
78700	(26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)
74000	(surface tension, Kinoshita et al. 1958)
70000	(titration, Petriris & Geankopolis 1959)
75600*	(20°C, synthetic method, measured range 0–125°C, von Erichsen 1962)
77800	(shake flask-GC, Korenman et al. 1974, 1975)
74000*	(shake flask-colorimetric analysis, De Santis et al. 1976)
70000*	(29.8°C, shake flask-refractometry, measured range 29.8–124.6°C, Aoki & Moriyoshi 1978)
63300	(generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
77000	(Verschuereen 1983; Howard 1990)
74000*	(recommended, IUPAC solubility series, temp range 10–110°C, Barton 1984)
74500	(selected, Riddick et al. 1986)

80300*	(20°C, shake flask-GC/TC, measured range 0–90.8°C, Stephenson & Stuart 1986)
74600	(selected, Yaws et al. 1990)
65720	(shake flask-GC, Li et al. 1992)
71230	(shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

800*	(24.0°C, static method, measured range 15.1–117.6°C, Kahlbaum 1898)
904*	(24.98°C, modified isoteniscope method, measured range 24.98–101.16°C, Butler et al. 1935)
$\log(P/\text{mmHg}) = 40.2105 - 4100/(T/K) - 10.35 \cdot \log(T/K)$; temp range 25–110°C (isoteniscope measurements, Butler et al. 1935)	
819	(saturated vapor density-gas saturation, Puck & Wise 1946)
667*	(20°C, summary of literature data, temp range –1.20 to 117°C, Stull 1947)
$\log(P/\text{mmHg}) = 8.27488 - 1873.9/(230 + t/^\circ\text{C})$ (Antoine eq., Dreisbach & Martin 1949)	
10274*	(64.56°C, measured range 64.56–117.56°C, Brown & Smith 1959)
820	(calculated-Antoine eq., Reid & Sherwood 1966)
733*	(22.6°C, ebulliometry-differential thermal analysis, measured range 22.6–117.8°C, Kemme & Kreps 1969)
$\log(P/\text{mmHg}) = 7.42117 - 1351.555/(179.810 + t/^\circ\text{C})$; temp range 22.6–117.8°C, or pressure range 5.5–766 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)	
910*	(comparative ebulliometry, measured range 78.558–125.686°C, Ambrose & Sprake 1970)
$\log(P/\text{Pa}) = 6.41435 - 1262.767/(T/K - 104.445)$; restricted temp range 78.558–100.74°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)	
$\log(P/\text{Pa}) = 6.54743 - 1338.769/(T/K - 96.108)$; temp range 78.558–125.686°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)	
864	(Hoy 1970)
948*	(298.11 K, measured range 283.10–323.12 K, Geiseler et al. 1973)
$\log(P/\text{mmHg}) = [-0.2185 \times 10970.5/(T/K)] + 8.929597$; temp range –1.2 to 277°C (Antoine eq., Weast 1972–73)	
868*	(24.96°C, vapor-liquid equilibrium data, temp range 281.1–323.12 K, Gmehling et al. 1982)
586, 1333	(20°C, 30°C, quoted, Verschueren 1983)
890	(interpolated-Antoine eq., Boublik et al. 1984)
$\log(P/\text{kPa}) = 6.54068 - 1335.018/(176.654 + t/^\circ\text{C})$; temp range 78.56–125.7°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)	
$\log(P/\text{kPa}) = 6.71950 - 1428.939/(185.552 + t/^\circ\text{C})$; temp range 41.5–108.8°C (Antoine eq. from reported exptl. data Kahlbaum 1898, Boublik et al. 1984)	
$\log(P/\text{kPa}) = 6.66896 - 1405.473/(183.866 + t/^\circ\text{C})$; temp range 64.5–117.56°C (Antoine eq. from reported exptl. data of Brown & Smith 1959, Boublik et al. 1984)	
$\log(P/\text{kPa}) = 6.7666 - 1460.309/(189.211 + t/^\circ\text{C})$; temp range 22.6–117.8°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)	
936	(Daubert & Danner 1985)
824	(interpolated-Antoine eq., Dean 1985)
$\log(P/\text{mmHg}) = 7.47680 - 1362.39/(178.77 + t/^\circ\text{C})$; temp range 15–131°C (Antoine eq., Dean 1985, 1992)	
910	(selected, Riddick et al. 1986)
$\log(P/\text{kPa}) = 6.54743 - 1338.769/(177.042 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)	
$\log(P_L/\text{kPa}) = 6.41661 - 1264.515/(-104.202 + T/K)$; temp range 376–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)	
$\log(P_L/\text{kPa}) = 6.54172 - 1336.026/(-96.348 + T/K)$; temp range 323–413 K (Antoine eq.-II, Stephenson & Malanowski 1987)	
$\log(P_L/\text{kPa}) = 7.05559 - 1738.4/(-46.544 + T/K)$, temp range: 413–550 K, (Antoine eq.-III, Stephenson & Malanowski 1987)	
$\log(P_L/\text{kPa}) = 8.9241 - 2697/(T/K)$; temp range 209–251 K (Antoine eq.-IV, Stephenson & Malanowski 1987)	
$\log(P_L/\text{kPa}) = 6.41594 - 1264.106/(-104.251 + T/K)$; temp range 376–397 K (Antoine eq.-V, Stephenson & Malanowski 1987)	
$\log(P_L/\text{kPa}) = 6.54723 - 1339.093/(-96.03 + T/K)$; temp range 351–397 K (Antoine eq.-VI, Stephenson & Malanowski 1987)	

- 905* (298.11 K, static method-Hg manometer, measured range 283.10–323.12 K, Gracia et al. 1992)
 998 (calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 39.6673 - 4.0017 \times 10^3/(T/K) - 10.295 \cdot \log(T/K) - 3.2572 \times 10^{-10} \cdot (T/K) + 8.6672 \times 10^{-7} \cdot (T/K)^2$;
 temp range 184–563 K (vapor pressure eq., Yaws 1994)
 933* (static method-manometer, measured range 278.15–323.15 K, Garriga et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.866 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 0.731 (entrainment method-GC, Burnett 1963)
 0.892 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 0.860; 0.964; 1.057 (exptl.; calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.80* (headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 0.860 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 4.024* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln(K_{\text{AW}}) = -10.2 + 5234/(T/K)$; temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)
 0.880 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 0.868 (wetted-wall column-GC, Altschuh et al. 1999)
 1.214 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 12.141 - 5982.0/(T/K)$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)
 0.53 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 6.600 - 3009/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.83 (shake flask-CR, Collander 1951)
 0.84 (calculated- π constant, Hansch et al. 1968)
 0.88 (Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Leo 1985)
 0.84, 0.86; 0.84 (calculated-fragment const.; calculated- π constant, Rekker 1977)
 0.89 (Hansch & Leo 1979)
 0.955 (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)
 1.02 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
 0.80 (calculated by Rekker's method, Hanai et al. 1981)
 0.79 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 0.76 (calculated from measured activity coeff. γ , Wasik et al. 1981)
 0.93 (shake flask-RC, Cornford 1982)
 0.80 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 0.87 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 0.79 (generator column-GC, Schantz & Martire 1987)
 0.80 (calculated from measured activity coeff., γ , Schantz & Martire 1987)
 0.87 (calculated- γ from UNIFAC, Banerjee & Howard 1988)
 0.823, 0.84 (calculated-CLOGP, calculated-M.O. indices, Bodor et al. 1989)
 0.84 (recommended, Sangster 1989, 1993)
 0.87 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)
 0.89 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
 0.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 4.19 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- −0.439 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC} :

1.85	(calculated- K_{OW} , Lyman et al. 1982)
0.64	(calculated-MCI χ , Gerstl & Helling 1987)
0.50	(soil, quoted exptl., Meylan et al. 1992)
0.39	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
0.50	(calculated- K_{OW} , Kollig 1993)
0.50	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate $k = 2.538 \times 10^{-4} \text{ mol m}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate $k = (50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^\circ\text{C}$ (Gückel et al. 1973);
estimated half-lives, $t_{1/2} \sim 2.4 \text{ h}$ in streams, $t_{1/2} \sim 3.9 \text{ h}$ in rivers and $t_{1/2} \sim 125.9 \text{ h}$ in lakes (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k = 2.2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ for the reaction with $1 \times 10^{-17} \text{ M}$ hydroxyl radical in water with $t_{1/2} \sim 1 \text{ yr}$ (Anbar & Neta 1967; quoted, Howard 1990)

photooxidation $t_{1/2} = 2602\text{--}104000 \text{ h}$ in water, based on measured rate constant for reaction with OH radical in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991)

$k_{OH} = 6.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K (relative rate method, Campbell et al. 1976)

photooxidation $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$t_{1/2} = 6.5 \text{ h}$ for the vapor phase reaction with photochemically produced NO radical in the atmosphere (Dilling et al. 1976; quoted, Howard 1990)

$k_{OH} = 4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k = 0.58 \pm 0.06 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0-6.0 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 6.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 7.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

photooxidation $t_{1/2} = 8.8\text{--}87.7 \text{ h}$ in air, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

estimated half-life of 2.3 d for the vapor phase reaction with photochemically produced OH radical in the atmosphere (GEMS 1986; quoted, Howard 1990)

$k_{OH}(\text{exptl}) = 7.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{OH}(\text{calc}) = 6.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = (8.31 \pm 0.63) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{OH}(\text{exptl}) = 8.31 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k(\text{soln}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987b)

$k_{OH} = 8.31 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = (7.2 - 8.31) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292-296 K (review, Atkinson 1989)

$k_{OH} = 8.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1990)

$k_{OH} = (7.80 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (8.56 \pm 0.70) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 8.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on unacclimated freshwater grab sample data (Hammerton 1955) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);

$k = 84.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$, average rate of biodegradation based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}$ (aq. anaerobic) = 96–1296 h, based on acclimated screening test data (Chou et al. 1979; selected, Howard et al. 1991) and aqueous aerobic biodegradation half-life (Howard et al. 1991);

k (calc) = $(0.959 \pm 0.063) \times 10^2 \text{ h}^{-1}$ by activated sludge (Yonezawa & Urushigawa 1979)

$k = 0.035\text{--}0.046 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 6.5 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976);

$t_{1/2}$ (calc) = 1.2 d for the atmospheric reaction with $1 \times 10^{-6} \text{ molecules/cm}^3$ of OH radical (Howard 1990);

photooxidation $t_{1/2} = 8.8\text{--}87.7 \text{ h}$, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; selected Howard et al. 1991).

Surface water: $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated freshwater grab sample data (Hammerton 1955; selected, Howard et al. 1991) and aqueous screening test data (Bridie et al. 1979; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 2602\text{--}104000 \text{ h}$, based on measured rate constant for reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991);

estimated volatilization half-lives, $t_{1/2} = 2.4 \text{ h}$ in streams, $t_{1/2} = 3.9 \text{ h}$ in rivers and $t_{1/2} = 125.9 \text{ h}$ in lakes (Lyman et al. 1982; quoted, Howard 1990).

Groundwater: $t_{1/2} = 48\text{--}1296 \text{ h}$, based on estimated aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.5.1

Reported aqueous solubilities of 1-butanol at various temperatures

1.

Fühner 1924		Hill & Malisoff 1926		Jones 1929		Mueller et al. 1931	
synthetic method		volumetric method		synthetic method		vapor liquid equilibrium	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	104500	5	95500	0	91000	0	95500
10	90000	10	89100	20.0	64000	15	83000
20	79000	15	82100	40.0	60300	30	70800
30	71000	20	78100	60.0	60000	45	65000
40	65500	25	73500	65.0	60300	60	65200
50	63500	30	70800	80.0	64000	75	68000
60	63500	35	68300	100.0	82000	90	78000
70	65500	40	66000	107.72	97900	105	98000
80	70000	50	64600	110.0	102000		
90	78000	60	65200	120.0	147000		
100	90500	70	67300				
110	10900	80	68900				
		97.9	87400				
		114.5	127300				
		116.9	134600				
		123.3	197300				
		125.15	304400				

(Continued)

TABLE 11.1.1.5.1 (Continued)

2.

von Erichsen 1952		Aoki & Moriyoshi 1978		Barton 1984		Stephenson & Stuart 1986	
synthetic method		shake flask-refractometry		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
at 1atm							
0	103200	29.8	70000	0	104000	0	103300
10	86800	49.6	69000	5	96000	9.6	89800
20	75600	59.5	75000	10	89000	20.0	80300
30	70600	69.5	67000	15	82000	30.8	70700
40	67200	89.5	75000	20	78000	40.1	67700
50	65500	99.3	95000	25	74000	50.0	65400
69	65200	106.9	106000	30	71000	60.1	63500
70	66700	109.8	110000	35	68000	70.2	67300
80	69000	118.1	145000	40	66000	80.1	70400
90	75000	119.1	172000	50	64000	90.8	72600
100	88200	122.1	182000	60	65000		
110	110500	122.7	189000	70	67000		
120	154500	123.9	218000	75	69000		
125	235000	124.3	247000	80	70000		
		124.6	279000	85	73000		
				90	77000		
				95	83000		
				100	91000		
				105	100000		
				110	111000		
				115	130000		
De Santis et al. 1976							
shake flask-colorimetry							
20	80000						
30	79400						
40	66000						

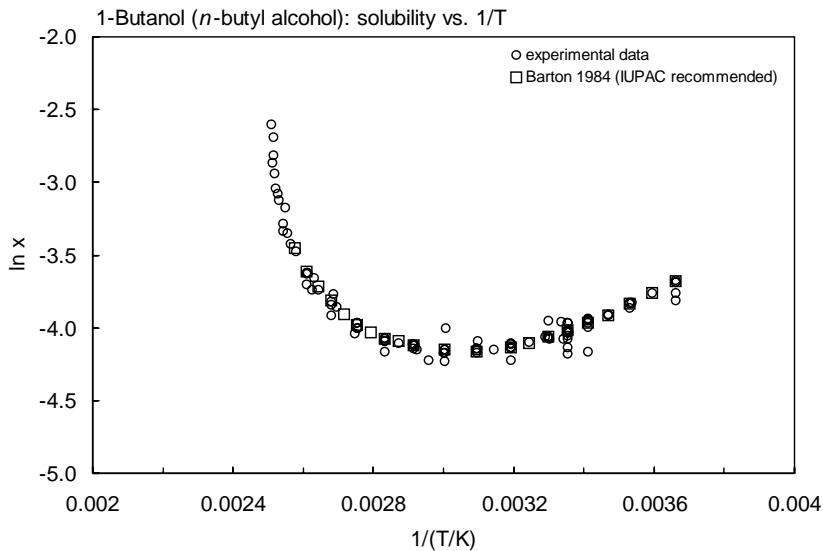


FIGURE 11.1.1.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-butanol.

TABLE 11.1.1.5.2

Reported vapor pressures of 1-butanol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/\{(T/K) - C\} & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Kahlbaum 1898		Butler et al. 1935		Stull 1947		Brown & Smith 1959	
static method		isoteniscope method		summary of literature data			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
41.5	2866	24.98	904	-1.20	133.3	64.56	10274
44.3	3200	40.0	1276	20.0	666.6	64.74	10371
46.2	3466	45.03	1800	30.2	1333	70.15	13668
48.6	4133	50.08	4593	41.5	2666	75.39	17692
50.1	4400	60.11	8091	53.4	5333	79.00	20982
52.0	5066	70.29	13732	60.3	7999	79.02	21022
55.0	5999	80.58	22465	70.1	13332	89.14	33160
60.2	7999	90.83	35544	84.3	26664	97.33	46859
64.3	9999	101.16	77140	100.8	53329	103.3	59548
69.8	13332			117.5	101325	108.23	72038
78.1	19998	bp/°C	117.71			113.26	86855
84.3	26664	D ²⁵	0.8059	mp/°C	-79.9	117.56	131371
89.4	33330						
93.7	39997	eq. 4	P/mmHg				
97.4	46663	A	40.2105				
100.0	53329	B	4100				
103.7	59995	C	10.35				
106.3	66661						
108.8	73327	$\Delta H_v(\text{kJ mol}^{-1}) = 52.84$ at 25°C					

2.

Kemme & Kreps 1969		Ambrose & Sprake 1970		Geiseler et al. 1973		Gmehling et al. 1982	
differential thermal analysis		comparative ebulliometry		Z. Phys. Chem. 254, 261		V-L equil. data collection	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
22.6	733.3	78.558	20413	283.10	309	283.10	269
30.9	1373	84.243	26518	288.13	457	288.13	405
36.2	1973	89.212	33045	293.12	663	293.12	599
40.7	2613	93.662	39973	298.11	948	298.11	868
48.2	4133	97.357	46601	303.11	1335	303.11	1241
52.4	5280	100.743	53450	308.10	1856	308.10	1744
58.3	7373	103.636	59932	313.08	2545	313.08	2416
65.8	10852	106.367	66630	318.11	3457	318.11	3309
73.5	16185	108.884	73332	323.12	4640	323.12	4473
85.1	27731	111.162	79856				
93.8	40463	113.429	86807	ref. from	Gracia 1989		
196.5	67594	115.324	92996				

(Continued)

TABLE 11.1.1.5.2 (Continued)

Kempe & Kreps 1969		Ambrose & Sprake 1970		Geiseler et al. 1973		Gmehling et al. 1982	
differential thermal analysis		comparative ebulliometry		Z. Phys. Chem. 254, 261		V-L equil. data collection	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa	T/K	P/Pa
117.8	102125	117.413	100142				
		119.193	106702				
Antoine eq.		120.939	113410				
eq. 2	P/mmHg	122.564	119943				
A	7.42117	124.115	126625				
B	1351.864	125.686	133323				
C	179.810						

3.

Gracia et al. 1992		Garriga et al. 2002	
static method-Hg manometer		static method-manometer	
T/K	P/Pa	T/K	P/Pa
283.10	265	278.15	192
288.13	411	283.15	230
293.12	613	288.15	453
298.11	905	293.15	635
303.11	1315	298.15	933
308.10	1831	303.15	1315
313.08	2522	308.15	1827
318.11	3420	313.15	2518
323.12	4600	318.15	3429
		323.15	4586
Antoine eq.			
eq. 3a	P/kPa		
A	12.12863		
B	2039.057		
C	132.925		

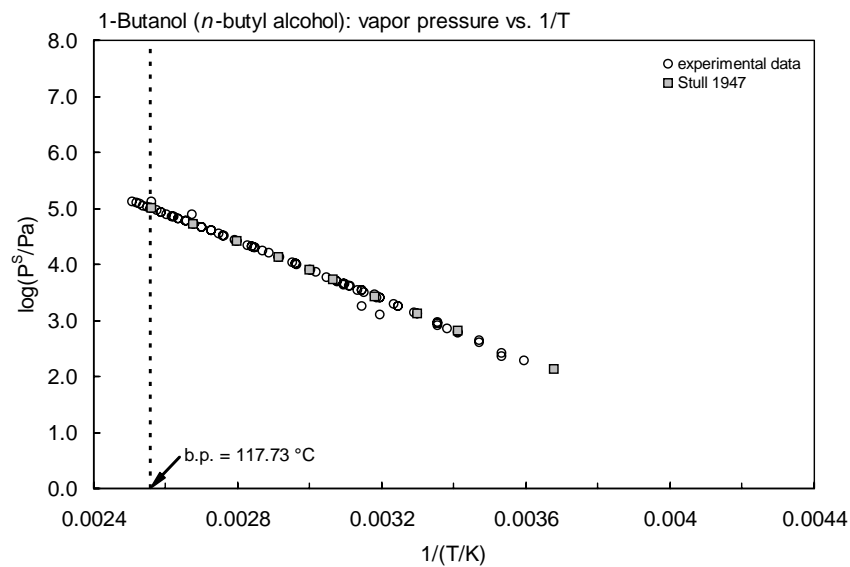


FIGURE 11.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 1-butanol.

TABLE 11.1.1.5.3
Reported Henry's law constants of 1-butanol at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/\text{atm}) = A - B/(T/K)$$
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$
$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

$$(1)$$
$$(2)$$
$$(3)$$
$$(4)$$
$$(5)$$

$$(1a)$$
$$(2a)$$
$$(4a)$$

Snider & Dawson 1985		Kolb et al. 1992	
gas stripping-GC		equilibrium headspace-GC	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
0	0.0873	40	4.024
25	0.800	60	11.64
		70	19.81
		80	29.69
enthalpy of transfer: ΔH/(kJ mol ⁻¹) = 58.576		eq. 2a	1/K _{AW}
		A	-10.2
		B	5234

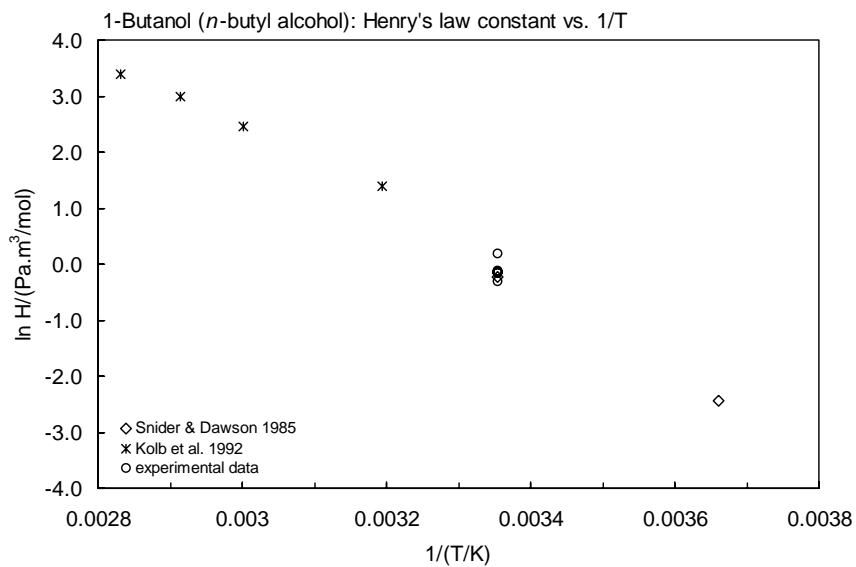
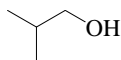


FIGURE 11.1.1.5.3 Logarithm of Henry's law constant versus reciprocal temperature for 1-butanol.

11.1.1.6 Isobutanol (*i*-Butyl alcohol)

Common Name: Isobutanol

Synonym: isobutyl alcohol, 2-methyl-1-propanol, *i*-butyl alcohol

Chemical Name: isobutanol, isobutyl alcohol, 2-methyl-1-propanol

CAS Registry No: 78-83-1

Molecular Formula: $C_4H_{10}O$, $(CH_3)_2CHCH_2OH$

Molecular Weight: 74.121

Melting Point ($^{\circ}C$):

−101.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

1087.89 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8018 (Weast 1982–83)

0.8016, 0.7978 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.5 ($20^{\circ}C$, calculated-density)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.32 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

100140 ($18^{\circ}C$, shake flask-turbidity, Fühner 1924)

85000 ($20^{\circ}C$, Seidell 1941)

75600 (shake flask-interferometry, Donahue & Bartell 1952)

94000 (shake flask-colorimetric, De Santis et al. 1976)

95000 ($18^{\circ}C$, Verschueren 1983)

76270 (IUPAC recommended, Barton 1984)

100000 (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1541* ($24.98^{\circ}C$, modified isoteniscope method, measured range 25 – $90^{\circ}C$, Butler et al. 1935)

$\log (P/mmHg) = 43.5513 - 4185/(T/K) - 11.50 \cdot \log (T/K)$; temp range 25 – $100^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

1648 (interpolated-regression of tabulated data, Stull 1947)

1333* ($21.7^{\circ}C$, summary of literature data, temp range -9.0 to $108^{\circ}C$, Stull 1947)

1527* (comparative ebulliometry, measured range 343.044 – $388.733\ K$, Ambrose & Sprake 1970)

$\log (P/Pa) = 6.35383 - 1194.628/(T/K - 106.291)$; restricted temp range 343 – $367.4\ K$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log (P/Pa) = 6.50091 - 1275.197/(T/K - 97.363)$; temp range 343 – $388.8\ K$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

$\log (P/mmHg) = [-0.2185 \times 10936.0/(T/K)] + 9.1138032$; temp range -9.0 to $241^{\circ}C$ (Antoine eq., Weast 1972–73)

1527 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.50091 - 1295.197/(t/^{\circ}C + 175.787)$, temp range not specified (Riddick et al. 1986)

$\log (P_L/kPa) = 6.34528 - 1190.463/(-106.712 + T/K)$; temp range 369 – $389\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.49241 - 1271.027/(-97.758 + T/\text{K})$; temp range 313–411 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.05055 - 1511.48/(-81.634 + T/\text{K})$; temp range 381–524 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.8507 - 2875/(T/\text{K})$; temp range 202–243 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.34606 - 1190.8481/(-106.673 + T/\text{K})$; temp range 369–389 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.50104 - 1275.669/(-97.269 + T/\text{K})$; temp range 342–389 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.27047 - 1147.676/(-111.933 + T/\text{K})$; temp range 383–416 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 109.2803 - 6.306 \times 10^3/(T/\text{K}) - 36.947 \cdot \log(T/\text{K}) + 1.4462 \times 10^{-2} \cdot (T/\text{K}) - 3.948 \times 10^{-13} \cdot (T/\text{K})^2$;
 temp range 165–548 K (vapor pressure eq., Yaws 1994)
 1500 (selected, Mackay et al. 1992, 1995)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

1.20	(measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
1.214	(exptl.- C_W/C_A , Hine & Mookerjee 1975)
1.159. 1.057	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
0.992	(headspace-GC, Snider & Dawson 1985)
1.186	(calculated-MCI χ , Nirmalakhandan & Speece 1988b)
1.84	(solid-phase microextraction SPME-GC, Bartelt 1997)
2.73	(gas stripping-GC, Shiu & Mackay 1997)
0.892	(wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.83	(shake flask-CR, Collander 1951)
0.61	(calculated- π constant, Hansch et al. 1968)
0.64	(Leo et al. 1969)
0.65	(from Hansch & Dunn III unpublished result, Leo et al. 1971)
0.76	(shake flask-GC, Dillingham et al. 1973)
0.76	(shake flask, Hansch & Leo 1985; 1987)
0.76	(recommended, Sangster 1989, 1993)
0.76	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.80	(calculated-measured γ^∞ in pure octanol and vapor pressure P , Abraham et al. 2001)
------	--

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2}(\text{calc}) = 79.7$ h for evaporation from a model river of 1-m deep with a current of 3 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982; selected, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 201$ d to 22 yr in water, based on measured rate for the reaction with OH radical in water (Anbar & Neta 1967; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 0.24$ –2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

photooxidation $t_{1/2} = 9.96\text{--}99.6$ h in air, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: biodegradation rate constant $k = 0.015\text{--}0.020$ h⁻¹ in 30 mg/L activated sludge after a time lag of 5–10 h (Urano & Kato 1986)

$t_{1/2}$ (aq. aerobic) = 43–173 h, based on river die-away data for one sample of water from one river (Hammerton 1955; selected, Howard et al. 1991)

$t_{1/2}$ (aq. anaerobic) = 172–692 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation half-life of 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976); photodecomposition $t_{1/2} = 3.5$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976); photooxidation $t_{1/2} = 9.96\text{--}99.6$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 201$ d to 22 yr, based on measured rate for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard et al. 1991); $t_{1/2} = 43\text{--}173$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 86\text{--}346$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 43\text{--}173$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

biota:

TABLE 11.1.1.6.1

Reported vapor pressures of isobutanol at various temperatures and the coefficients for the equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Butler et al. 1935		Stull 1947		Ambrose & Sparke 1970	
isoteniscope method		summary of literature data		comparative ebulliometry	
t/ ^o C	P/Pa	t/ ^o C	P/Pa	T/K	P/Pa
24.98	1541	−9.0	133.3	343.044	20457
40.0	2196	11.0	666.6	348.552	26554
45.03	2985	21.7	1333	353.357	33057
50.08	7415	32.4	2666	357.674	39994
60.11	12778	44.1	5333	361.213	46532
70.29	21292	51.7	7999	364.531	53442
80.58	34184	61.5	13332	367.356	59959
90.83	53036	75.9	26664	369.965	66546
		91.4	53329	372.439	73326
bp/ ^o C	82.39	108.0	101325	374.696	79983
D ²⁵	0.7812			376.846	86765

(Continued)

TABLE 11.1.1.6.1 (Continued)

Butler et al. 1935		Stull 1947		Ambrose & Sparke 1970	
isoteniscope method		summary of literature data		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
		mp/°C	−108	378.739	93121
eq. 4	P/mmHg			380.718	100153
A	43.5513			382.476	106746
B	4185			384.166	113.417
C	11.50			385.775	120072
$\Delta H_v/(\text{kJ mol}^{-1}) = 51.63$				387.252	126441
at 25°C				388.773	133283

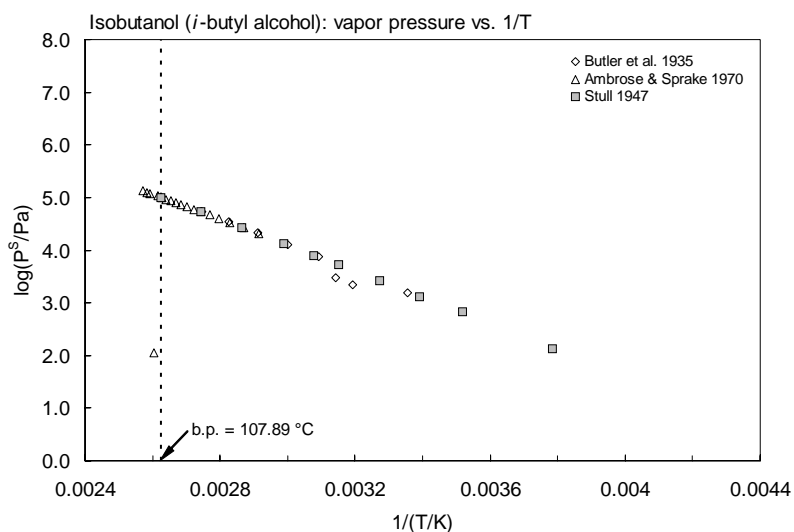
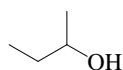


FIGURE 11.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for isobutanol.

11.1.1.7 *sec*-Butyl alcohol

Common Name: *sec*-Butyl alcohol

Synonym: 2-butyl alcohol, 2-butanol, methylethylcarbinol

Chemical Name: 2-butanol, *sec*-butyl alcohol

CAS Registry No: 78-92-2

Molecular Formula: C₄H₁₀O, CH₃CH₂CHOHCH₃

Molecular Weight: 74.121

Melting Point (°C):

−88.5 (Lide 2003)

Boiling Point (°C):

99.51 (Lide 2003)

Density (g/cm³ at 20°C):

0.8063 (Weast 1982–83)

0.8065, 0.8024 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

91.9 (20°C, calculated-density)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

200000 (20°C, synthetic method, Jones 1929)

185000 (20°C, shake flask, Evans 1936)

198000* (20°C, shake flask-refractometer, measured range 20–85°C, Morachevskii & Popovich 1965)

177000, 165000 (25, 35°C, shake flask-titration, Ratouis & Dodé 1965)

202000* (20°C, equilibrium pressure cell/shake flask-refractometric method, measured range 10–110°C, pressure range 1–800 atm, Moriyoshi et al. 1975)

225000 (shake flask-colorimetric analysis, De Santis et al. 1976)

130000 (shake flask-refractometric method, Becke & Quitzch 1977)

187000* (equilibrium pressure vessel/shake flask-GC, measured range 265–372 K, pressure range 0.1–75 MPa, Bozdog & Lamb 1983)

181000* (recommended, IUPAC solubility series, temp range 10–110°C, Barton 1984)

196000* (20°C, shake flask-GC/TC, measured range 0–90.2°C, Stephenson & Stuart 1986)

175340* (25.28°C, shake flask-laser scattering technique, measured range 276.94–386.6 K, Ochi et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2286* (modified isoteniscope method, measured range 25–91°C. Butler et al. 1935)

log (P/mmHg) = 43.4800 − 4110/(T/K) − 11.50 · log (T/K); temp range 25–90°C (isoteniscope measurements, Butler et al. 1935)

2266* (interpolated-regression of tabulated data, temp range −12.2 to 99.5°C, Stull 1947)

33031* (73.392°C, ebulliometry, measured range 73.392–107.146°C, Biddiscombe et al. 1954)

10610* (49.730°C, measured range 49.730–99.410°C, Brown et al. 1969)

2317* (comparative ebulliometry, measured range 67.723–107.743°C, Ambrose & Sprake 1970)

log (P/Pa) = 6.26852 − 1126.667/(T/K − 108.361); restricted temp range 67.7–83.34°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 6.86618 − 1360.131/(T/K − 75.558); temp range 67.723–107.743°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

2357 (Hoy 1970)

$\log(P/\text{mmHg}) = [-0.2185 \times 10712.3/(T/K)] + 9.096778$; temp range -12.2 – 251°C (Antoine eq., Weast 1972–73)
1600, 3200 (20°C, 30°C, Verschueren 1983)

2200, 2190, 2275 (extrapolated-Antoine equations, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.35079 - 1169.924/(169.731 + t/^\circ\text{C})$; temp range 67.7 – 107.14°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.32690 - 1157.363/(168.32 + t/^\circ\text{C})$; temp range 72.39 – 107.15°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1954, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.47826 - 1235.4/(176.82 + t/^\circ\text{C})$; temp range 49.73 – 99.41°C (Antoine eq. from reported exptl. data of Brown et al. 1969, Boublik et al. 1984)

2438 (calculated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.47431 - 1314.31/(186.55 + t/^\circ\text{C})$; temp range 25 to 120°C (Antoine eq., Dean 1985, 1992)

2317 (selected, Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.35457 - 1171.893/(t/^\circ\text{C} + 169.955)$, temp range not specified (Riddick et al. 1986)

$\log(P_L/\text{kPa}) = 6.26823 - 1126.887/(-108.291 + T/K)$; temp range 359 – 381 K (Antoine eq-I., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.34976 - 1169.754/(-103.388 + T/K)$; temp range 3039 – 403 K (Antoine eq-II., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.74369 - 735.87/(-176.795 + T/K)$; temp range 372 – 5241 K (Antoine eq-III., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 7.50959 - 1751.931/(-52.906 + T/K)$; temp range 210 – 303 K (Antoine eq-IV., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.2663 - 1125.853/(-108.414 + T/K)$; temp range 359 – 380 K (Antoine eq-V., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.35314 - 1171.484/(-103.199 + T/K)$; temp range 340 – 379 K (Antoine eq-VI., Stephenson & Malanowski 1987)

2440, 997 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 49.4476 - 4.2487 \times 10^3/(T/K) - 13.793 \cdot \log(T/K) + 6.2736 \times 10^{-11} \cdot (T/K) + 2.1988 \times 10^{-6} \cdot (T/K)^2$;
temp range 158 – 536 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.040 (measured partial pressure/mole fraction x at dilute concn, Butler 1935)

1.033 (exptl., Hine & Mookerjee 1975)

1.60, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.918* (headspace-GC, measured range 0 – 25°C , Snider & Dawson 1985)

1.107 (calculated-MCI χ , Nirmalakhandan & Speece 1988b)

0.604 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{\text{AW}} = 6.734 - 3031/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.61 (shake flask-GC, Hansch & Anderson 1967; Hansch et al. 1968)

0.74, 0.64 (calculated-f const., calculated- π const., Rekker 1977)

0.81 (HPLC-RT correlation, Yonezawa & Urushigawa 1979)

0.87 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

0.65 (recommended, Sangster 1989)

0.61 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section:

3.99* (20.29°C , from GC determined γ^∞ in octanol, measured range 20.29 – 50.28°C , Gruber et al. 1997)

3.80 (calculated from determined γ^∞ in octanol and vapor pressure, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 129$ d to 23 yr, based on measured rate for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 0.24$ – 2.4 h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 4.1 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for at 25°C with $t_{1/2} = 1.3$ d (Hendry & Kenley 1979; quoted, Mill 1982)

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 24$ – 168 h, based on river die-away studies (Hammerton 1955; selected, Howard et al. 1991) and aqueous anaerobic $t_{1/2} = 96$ – 672 h, based on estimated aqueous aerobic biodegradation half-life (selected, Howard et al. 1991);

average rate of biodegradation $k_B = 55.0 \text{ (mg COD g}^{-1} \text{ h}^{-1})$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.24$ – 2.4 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 4.0$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976);

photooxidation $t_{1/2} = 7.2$ – 72 h, based on measured rate constant for the reaction with OH radical in air (Edney & Corse 1986; selected, Howard et al. 1991);

calculated lifetimes of 1.3 d and 17 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000)

Surface water: $t_{1/2} = 24$ – 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ – 336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24$ – 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.7.1

Reported aqueous solubilities of sec-butyl alcohol at various temperatures

1.

Morachevskii & Popovich '65		Moriyoshi et al. 1975		Bozdag & Lamb 1983		Barton 1984	
shake flask-refractometry		shake flask-refractometry		equil. pressure cell-GC		IUPAC recommended	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
			at 1 atm		at 0.1 MPa		
20	198000	10	239000	–8	271000	10	239000
40	146000	20	202000	–6	266000	20	199000
60	140000	27	179000	–4	266000	25	181000
80	140000	40	149000	–3	263000	30	175000

(Continued)

TABLE 11.1.1.7.1 (Continued)

Morachevskii & Popovich '65		Moriyoshi et al. 1975		Bozdag & Lamb 1983		Barton 1984	
shake flask-refractometry		shake flask-refractometry		equil. pressure cell-GC		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
85	150000	50	132000	0	264000	35	163000
		60	128000	2	256000	40	155000
		70	129000	5	249000	50	140000
		80	138000	10	232000	60	142000
		90	155000	15	228000	70	138000
		100	183000	20	203000	80	143000
		110	239000	25	187000	90	158000
				30	171000	100	186000
						110	239000
		measured range 283–378 K		measured range 265–372 K			
		pressure range 1–800 atm		pressure range 0.1–75 MPa			
		full list of data see ref.		full list of data see ref.			

2.

Stephenson & Stuart 1986		Ochi et al. 1996			
shake flask-GC/TC		laser scattering technique			
t/°C	S/g·m ⁻³	T/K	mole frac. x	T/K	mole frac. x
0	260000	276.94	0.0738	362.51	0.0406
10	235000	278.13	0.0725	364.96	0.0421
20	196000	279.96	0.0705	370.41	0.0459
29.9	170000	284.94	0.0642	376.89	0.0530
40	151000	289.08	0.0590	379.76	0.0573
50	140000	290.58	0.0571	381.25	0.0621
60.3	134000	292.18	0.0553	383.23	0.0680
70.1	133000	295.15	0.0522	384.39	0.0751
80.1	136000	298.43	0.0491	385.63	0.0820
90.2	145000	301.48	0.0471	386.04	0.0908
		305.14	0.0452	386.23	0.0965
		309.16	0.0421	386.58	0.1050
		311.88	0.0406	386.65*	0.1151
		314.10	0.0393	*the upper critical solution point	
		321.88	0.0371		
		324.99	0.0361		
		332.50	0.0342		
		340.01	0.0342		
		349.30	0.0361		
		352.25	0.0371		
		360.81	0.0393		

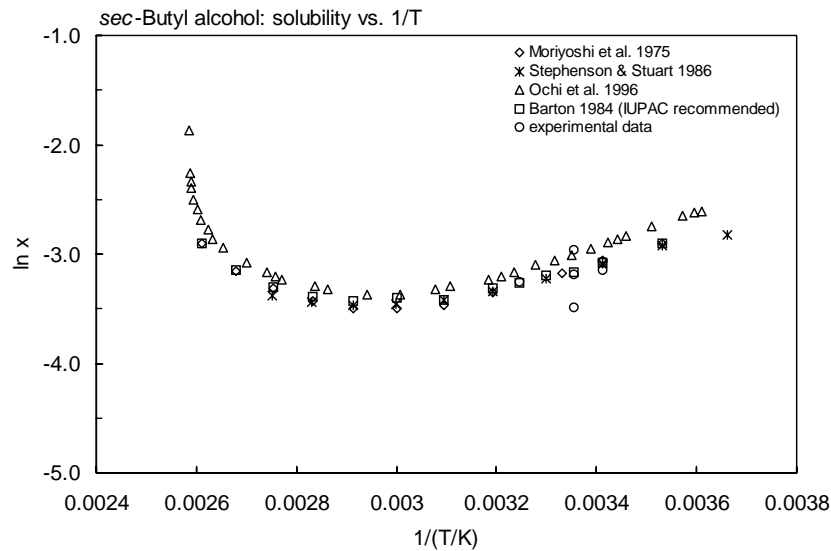


FIGURE 11.1.1.7.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for sec-butyl alcohol.

TABLE 11.1.1.7.2
Reported vapor pressures of sec-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)

log P = A – B/(C + t/°C)

log P = A – B/(C + T/K)

log P = A – B/(T/K) – C·log (T/K)

(1)

(2)

(3)

(4)

ln P = A – B/(T/K)

ln P = A – B/(C + t/°C)

(1a)

(2a)

1.

Butler et al. 1935		Stull 1947		Biddiscombe et al. 1954		Brown et al. 1969	
isoteniscope method		summary of literature data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	2286	–12.2	133.3	73.392	33031	49.730	10610
40.0	3272	7.20	666.6	76.600	39942	54.050	13402
45.03	4440	16.9	1333	80.131	46616	57.740	16271
50.08	10764	27.3	2666	83.340	53447	62.020	20198
60.12	18452	38.1	5333	86.112	39983	67.498	16382
70.3	29878	45.2	7999	88.693	66641	72.180	32861
80.59	47356	54.1	13332	91.068	73266	76.970	40792
90.84	72407	67.9	26664	93.303	80010	83.060	53067
		83.9	53329	95.394	86761	88.450	66274
bp/°C	99.95	99.5	101325	97.252	93093	94.160	83033
D ²⁵	0.8029			99.201	100155	99.410	101321
		mp/°C	–114.7	100.931	106774		
eq. 4	P/mmHg			120.611	113533		
A	43.4800			104.186	120168		
B	4110			105.647	126596		
C	11.50			107.146	133.471		
ΔH_v /(kJ mol ^{–1}) = 50.21							
at 25°C							

(Continued)

TABLE 11.1.1.7.2 (Continued)

2.

Ambrose & Sprake 1970

comparative ebulliometry

t/°C	P/Pa
67.723	26556
72.392	33031
76.601	39942
80.131	46616
83.340	53447
86.111	59984
88.693	66641
91.067	73284
93.303	81010
95.394	86759
97.253	93095
99.201	100154
100.931	106775
102.611	113530
104.186	120167
105.647	126593
107.143	133470

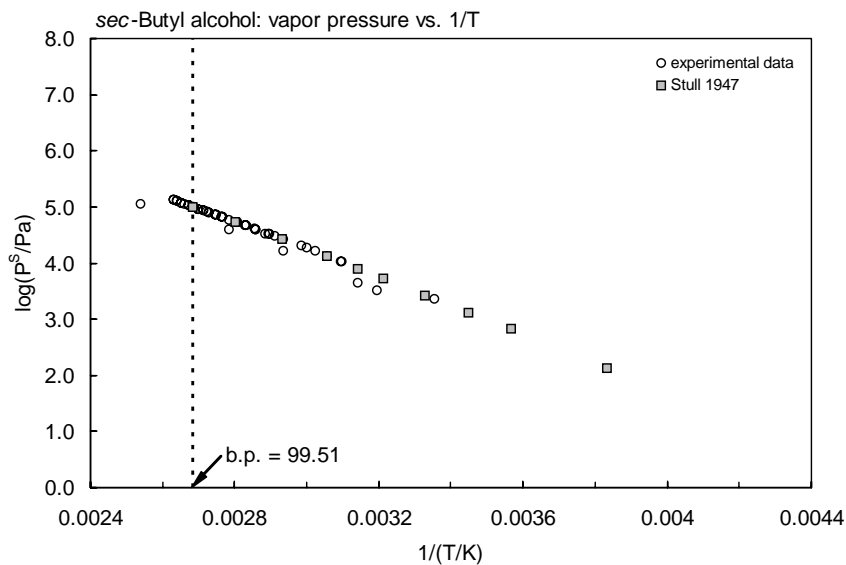


FIGURE 11.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for sec-butyl alcohol.

TABLE 11.1.1.7.3
Reported Henry's law constants and octanol-air partition coefficients of sec-butyl alcohol at various temperatures

Henry's law constant		log K _{OA}	
Snider & Dawson 1985		Gruber et al. 1997	
gas stripping-GC		GC det'd activity coefficient	
t/°C	H/(Pa m ³ /mol)	t/°C	log K _{OA}
0	0.0987	20.29	3.98
25	0.9180	30.3	3.68
		40.4	3.44
		50.28	3.22
enthalpy of transfer: ΔH/(kJ mol ⁻¹) = 58.576			

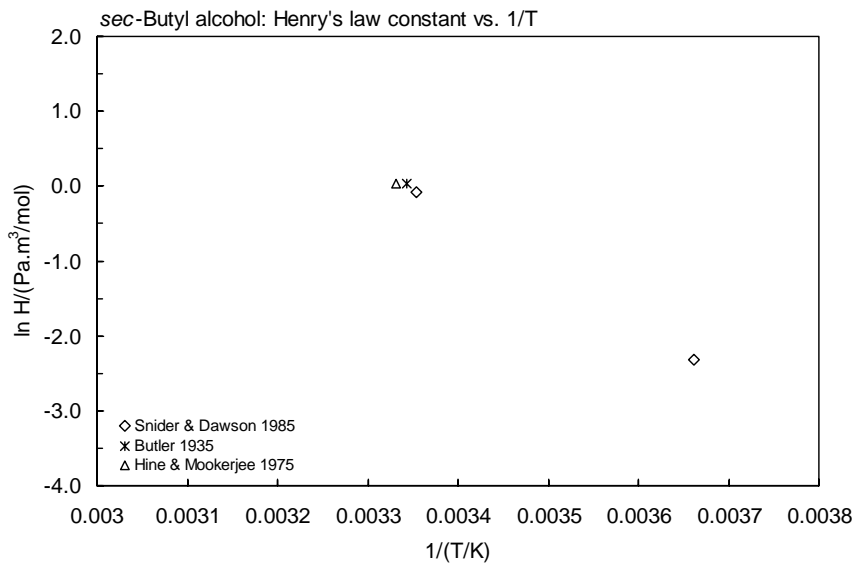


FIGURE 11.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for sec-butyl alcohol.

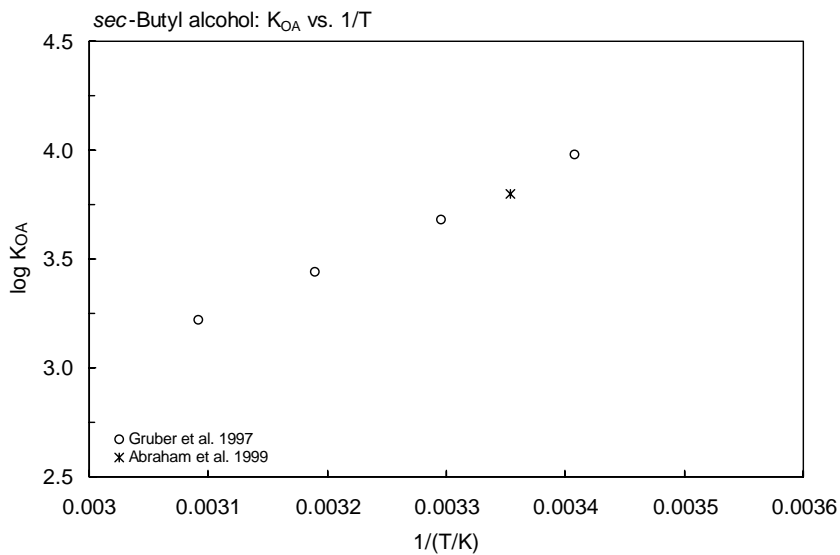


FIGURE 11.1.1.7.4 Logarithm of K_{OA} versus reciprocal temperature for sec-butyl alcohol.

11.1.1.8 *tert*-Butyl alcohol

Common Name: *tert*-Butyl alcohol

Synonym: 3-butanol, *t*-butyl alcohol, 2-methyl-2-propanol, trimethylcarbinol,

Chemical Name: *t*-butanol, *t*-butyl alcohol, 2-methyl-2-propanol

CAS Registry No: 75-65-0

Molecular Formula: C₄H₁₀O, (CH₃)₃COH

Molecular Weight: 74.121

Melting Point (°C):

25.69 (Lide 2003)

Boiling Point (°C):

82.4 (Lide 2003)

Density (g/cm³ at 20°C):

0.78581, 0.78086 (20°C, 25°C, Dreisbach & Martin 1949)

0.7883 (Weast 1982–83)

0.7858 (Dean 1985)

0.7812 (25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

94.2 (calculated-density, Rohrschneider 1973)

103.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.64 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

22.76, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming ΔS = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

miscible (Palit 1947; Riddick et al. 1986)

miscible (Barton 1984; Dean 1985; Howard 1990; Yaws et al. 1990)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5600* (static method/isoteniscope, measured range 20–90°C, Parks & Barton 1928)

5654* (24.98°C, modified isoteniscope method, measured range 30–80°C, Butler et al. 1935)

log (P/mmHg) = 43.2834 – 3935/(T/K) – 11.50·log (T/K); temp range 30–80°C (isoteniscope measurements, Butler et al. 1935)

5019* (interpolated-regression of tabulated data, temp range –20.4 to 82.9°C, Stull 1947)

log (P/mmHg) = 8.24380 – 1675.4/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

16500* (43.34°C, measured range 43.34–82.41°C, Dreisbach & Shrader 1949)

5637* (comparative ebulliometry, measured range 329.946–362.710 K, Ambrose & Sprake 1970)

log (P/Pa) = 6.24072 – 1049.320/(T/K – 107.724); restricted temp range 329.946–345.288 K (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/Pa) = 6.35648 – 1107.060/(T/K – 101.048); temp range 329.946–362.71 K (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)

log (P/mmHg) = [–0.2185 × 10413.2/(T/K)] + 9.193472; temp range –20.4 to 222.5°C (Antoine eq., Weast 1972–73)

5600 (Verschueren 1983; Howard et al. 1986)

5637 (selected, Riddick et al. 1986)

log (P/kPa) = 6.35648 – 1107.060/(t/°C + 172.102) temp not specified (Riddick et al. 1986)

log (P_L/kPa) = 6.22619 – 1042.416/(–108.5 + T/K); temp range 347–363 K (Antoine eq.-I, Stephenson & Malanowski 1987)

- $\log (P_L/\text{kPa}) = 6.35045 - 1104.341/(-101.315 + T/\text{K})$; temp range 299–375 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.27388 - 989.74/(-124.966 + T/\text{K})$; temp range 356–480 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.23125 - 1044.891/(-108.211 + T/\text{K})$, temp range: 347–363 K, (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.35498 - 1106.556/(-101.071 + T/\text{K})$; temp range 329–363 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.09542 - 975.944/(-116.864 + T/\text{K})$; temp range 357–461 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 1008, 5600 (calculated-solvatochromic parameters, quoted lit., Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 71.8181 - 4.9966 \times 10^3/(T/\text{K}) - 21.805 \cdot \log(T/\text{K}) + 1.9238 \times 10^{-8} \cdot (T/\text{K}) + 5.8247 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 299–506 K (vapor pressure eq., Yaws 1994)
 5610* (static method-manometer, measured range 298.15–323.15 K, Garriga et al. 2002)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.210 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
 1.214 (exptl., Hine & Mookerjee 1975)
 1.057, 1.057 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.460* (25°C headspace-GC, measured range 0–25°C, Snider & Dawson 1985)
 1.426 (calculated-MCI χ , Nirmalakhandan & Speece 1988b)
 0.917 (wetted-wall column-GC, Altschuh et al. 1999)
 0.907 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 8.467 - 3488/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.37 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1969)
 0.59 (HPLC-RT correlation, Yonezawa & Urushigawa 1979)
 0.35 (Hansch & Leo 1985)
 0.40 (calculated-solvatochromic parameters, Taft et al. 1985)
 0.39 (HPLC- k' correlation, Funasaki et al. 1986)
 0.34 (shake flask, Log P Database, Hansch & Leo 1987)
 0.35 (recommended, Sangster 1989)
 0.34 (calculated-UNIFAC activity coefficient, Dallos et al. 1993)
 0.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 3.50 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- −1.46 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.57 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated half-lives, $t_{1/2} = 51.6$ h in streams, $t_{1/2} = 65.37$ h in rivers and $t_{1/2} = 3104.3$ h in lakes were estimated by using Henry's law constant and assuming the wind velocity to be 3 m/s, the current velocities of the streams, rivers, and lakes 2, 1, and 0.01 m/s with depths of lakes 50 m and that of the streams and lakes 1 m deep (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 771 \text{ d to } 64500 \text{ yr}$, based on measured rate for the reaction with hydroxyl radical in water (Howard et al. 1991)

photooxidation $t_{1/2} > 9.9 \text{ d}$ (Darnall et al. 1976)

$k \sim 0.003 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2–6 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}}(\text{calc}) = 6.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 59\text{--}590 \text{ h}$, based on measured rate for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

$k_{\text{OH}}(\text{calc}) = 5.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{exptl}) = 1.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (1.08 \pm 0.11) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987a)

$k_{\text{OH}} = 1.07 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}^* = 1.07 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 243–440 K (flash photolysis-resonance fluorescence, Wallington 1988c)

$k_{\text{OH}}^* = 1.12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k(\text{aq.}) = 0.01 \text{ M}^{-1} \text{ s}^{-1}$ at pH 2.3, $k = 0.45 \text{ M}^{-1} \text{ s}^{-1}$ at pH 2.2, $k = 0.46 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.2 for direct reaction with ozone in water and 20°C, with $t_{1/2} = 390 \text{ d}$ at pH 7 (Yao & Haag 1991).

$k_{\text{OH}}(\text{calc}) = 0.53 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $30.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}(\text{aq. aerobic}) = 677\text{--}4320 \text{ h}$, based on river die-away studies; $t_{1/2}(\text{aq. anaerobic}) = 2400\text{--}12000 \text{ h}$, based on degradation rates in microcosm studies simulating anaerobic aquifers (Howard et al. 1991).

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 100 \text{ d}$ in natural waters (Capel & Larson 1995)

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} > 9.9 \text{ d}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 34.5 \text{ h}$ for 10 ppm in the air reacted with 5 ppm NO (Dilling et al. 1976);

photooxidation $t_{1/2} = 59\text{--}590 \text{ h}$, based on measured rate for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);

$t_{1/2} \sim 1.09 \text{ month}$ for the vapor phase reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1990).

Surface water: $t_{1/2} \sim 8.8 \text{ yr}$, based on rate constant $k = 2.5 \times 10^8 \text{ L/mol}\cdot\text{s}$ for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; quoted, Howard 1990);

$t_{1/2} = 672\text{--}4320 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

measured rate constant $k = 0.001 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2.3 and 20°C, with $t_{1/2} = 390 \text{ d}$ at pH 7 (Yao & Haag 1991)

$t_{1/2}(\text{aerobic}) = 28 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 100 \text{ d}$ in natural waters (Capel & Larson 1995)

Groundwater: $t_{1/2} = 1344\text{--}8640 \text{ h}$, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 360\text{--}4800 \text{ h}$, based on soil microcosm studies (Howard et al. 1991).

Biota:

TABLE 11.1.1.8.1

Reported vapor pressures of *tert*-butyl alcohol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Parks & Barton 1928		Butler et al. 1935		Stull 1947		Garriga et al. 2002	
static method/isoteniscope		isoteniscope method		summary of literature data		static method-manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
20	4080	24.98	5654*	−20.4	133.3	25	5610
25	5600	40.0	7753	−3.0	666.6	30	7685
30	7586	45.03	10423	5.5	1333	35	10347
35	10172	50.08	23705	14.3	2666	40	13787
40	13639	60.12	38850	24.5	5333	45	18143
45	17839	70.3	61648	31.0	7999	50	23578
50	23238	75.43	72927	39.8	13332	Ambrose & Sprake 1970 comparative ebulliometry	
55	29891	80.59	100112	52.7	26664		
60	38024		*solid	68.0	53329	T/K	P/Pa
65	47756	bp/°C	82.75	82.9	101325	329.946	33123
70	59635					333.931	40058
75	73754	eq. 4	P/mmHg	mp/°C	25.3	337.204	46623
80	90579	A	43.2834			340.225	53431
85	110164	B	3935			342.857	60007
90	132816	C	11.59			347.448	73160
$\Delta H_v/(\text{kJ mol}^{-1}) =$ at 25°C 45.56 at bp 39.66		$\Delta H_v/(\text{kJ mol}^{-1}) = 46.86$ at 25°C		Dreisbach & Shrader 1949		351.659	86911
				ebulliometry		355.146	99932
				t/°C	P/Pa	358.422	113545
				43.34	16500	362.710	133505
				61.82	42066	full list of data see ref.	
				72.49	67661		
				82.41	101325		

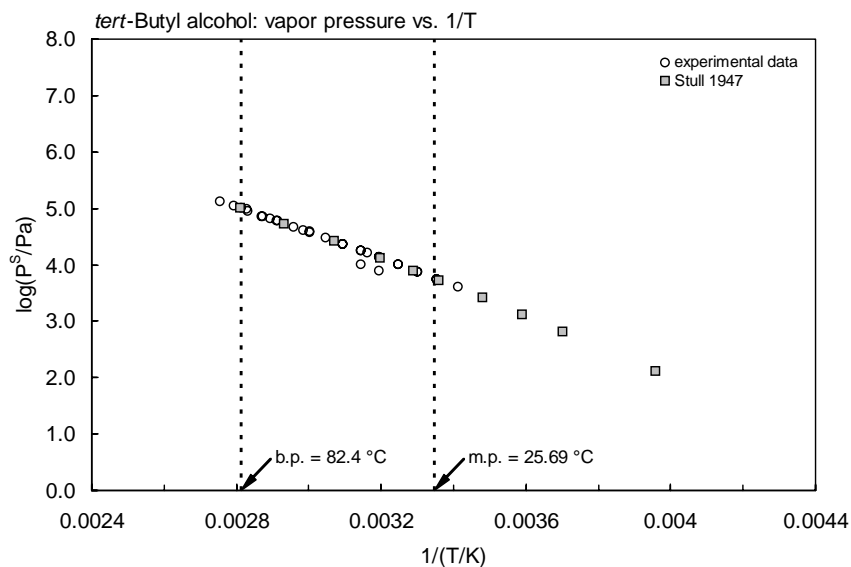


FIGURE 11.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for *tert*-butyl alcohol.

TABLE 11.1.1.8.2

Reported Henry's law constants of *tert*-butyl alcohol at various temperatures

Snider & Dawson 1985

gas stripping-GC

t/°C	H/(Pa m ³ /mol)
0	0.1135
25	1.4581

enthalpy of transfer:
 $\Delta H/(\text{kJ mol}^{-1}) = 66.944$

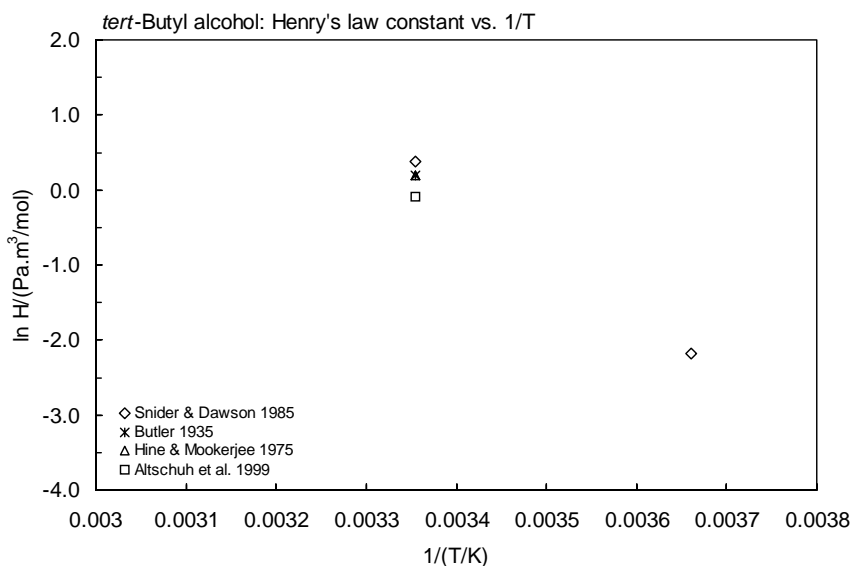
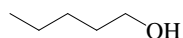


FIGURE 11.1.1.8.2 Logarithm of Henry's law constant versus reciprocal temperature for *tert*-butyl alcohol.

11.1.1.9 1-Pentanol (*n*-Amyl alcohol)

Common Name: 1-Pentanol

Synonym: amyl alcohol, *n*-butylcarbinol, 1-pentanol, *n*-pentyl alcohol, pentyl alcohol

Chemical Name: *n*-amyl alcohol, *n*-pentyl alcohol, 1-pentanol

CAS Registry No: 71-41-0

Molecular Formula: $C_5H_{12}O$, $CH_3CH_2CH_2CH_2CH_2OH$

Molecular Weight: 88.148

Melting Point ($^{\circ}C$):

−77.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

137.98 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.81253 ($25^{\circ}C$, Butler et al. 1935)

0.8144 (Weast 1982–83)

0.81445, 0.81080 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

108.0 (calculated-density, Lande & Banerjee 1981)

125.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

20.81 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.5 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

22080 (shake flask-interferometer, Butler et al. 1933)

21900* (volumetric method, measured range 20 – $30^{\circ}C$, Ginnings & Baum 1937)

22100 ($20^{\circ}C$, surface tension, Addison 1945)

23600 ($20^{\circ}C$, Seidell 1941)

27570 (shake flask-residue volume, Booth & Everson 1948)

15230 ($20^{\circ}C$, shake flask-turbidity, Laddha & Smith 1948)

25400 (shake flask-interferometry, Hansen et al. 1949)

23500* ($20^{\circ}C$, synthetic method, measured range 0 – $180^{\circ}C$, von Erichsen 1952)

22000 (shake flask-titration, Crittenden & Hixon 1954)

22140 (estimated, McGowan 1954)

22000 (surface tension, Kinoshita et al. 1958)

23800 (shake flask-GC, Korenman 1974, 1975)

21950 (Riddick & Bunger 1955)

18800 (shake flask-GC, Evans et al. 1978)

11720 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

22000* (recommended best value, IUPAC Solubility Data Series, temp range 0 – $180^{\circ}C$, Barton 1984)

22500* ($20.2^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.7^{\circ}C$, Stephenson et al. 1984)

20190 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

333* ($25^{\circ}C$, extrapolated-modified isoteniscope method, measured range 60 – $131^{\circ}C$, Butler et al. 1935)

- $\log (P/\text{mmHg}) = 46.4925 - 4580/(T/K) - 12.42 \cdot \log (T/K)$; temp range 60–131°C (isoteniscope measurements, Butler et al. 1935)
- 349* (interpolated-regression of tabulated data, temp range 13.6–138°C, Stull 1947)
- 286* (extrapolated-ebulliometry, measured range 33.9–138°C, Kemme & Kreps 1969)
- 573.3* (33.9°C, ebulliometry-differential thermal analysis, measured range 33.9–138°C, Kemme & Kreps 1969)
- $\log (P/\text{mmHg}) = 7.55787 - 1492.549/(181.529 + t/^{\circ}\text{C})$; temp range 33.9–138°C, or pressure range 4.3–765.4 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
- 293* (comparative ebulliometry, measured range 74.763–156°C, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 6.13796 - 1190.412/(T/K - 123.055)$; restricted temp range 74.763–128.665°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 6.30306 - 1286.333/(T/K - 111.843)$; temp range 74.763–128.665°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- 313 (calculated-Antoine eq., Riddick & Bunger 1970)
- $\log (P/\text{mmHg}) = [-0.2185 \times 12495.5/(T/K)] + 9.574342$; temp range 13.6–137.8°C (Antoine eq., Weast 1972–73)
- 189 (20°C, extrapolated-Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
- 373 (20°C, Verschueren 1983)
- 172, 250 (extrapolated-Antoine equations., Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.00024 - 1103.91/(138.221 + t/^{\circ}\text{C})$; temp range 165–240.65°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.31559 - 1292.273/(161.837 + t/^{\circ}\text{C})$; temp range 74.5–156°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
- 313 (extrapolated-Antoine eq., Dean 1985)
- $\log (P/\text{mmHg}) = 7.17758 - 1314.56/(168.11 + t/^{\circ}\text{C})$; temp range 37–138°C (Antoine eq., Dean 1985, 1992)
- 293 (selected, Riddick et al. 1986)
- $\log (P/\text{kPa}) = 6.30306 - 1286.333/(t/^{\circ}\text{C} + 161.307)$, temp range not specified (Riddick et al. 1986)
- $\log (P_L/\text{kPa}) = 6.14668 - 1195.924/(-122.348 + T/K)$; temp range 388–420 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.30990 - 1290.23/(-111.419 + T/K)$; temp range 347–429 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.1490 - 1197.233/(-122.194 + T/K)$; temp range 388–420 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.3975 - 1337.613/(-106.567 + T/K)$; temp range 326–411 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.28069 - 1277.413/(-112.34 + T/K)$; temp range 408–441 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- $\log (P/\text{mmHg}) = 71.2535 - 5.4977 \times 10^3/(T/K) - 21.366 \cdot \log(T/K) + 3.8108 \times 10^{-10} \cdot (T/K) + 5.0339 \times 10^{-6} \cdot (T/K)^2$; temp range 196–586 K (vapor pressure eq., Yaws 1994)
- 891 (40°C, vapor-liquid equilibrium VLE data, Rhodes et al. 1997)

Henry's Law Constant (Pa m³/mol):

- 1.324 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
- 1.271 (exptl., Hine & Mookerjee 1975)
- 1.426, 1.60 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 1.04 (calculated-P/C, Mackay & Yuen 1983)
- 1.017 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
- 1.271 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 1.236 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
- 1.60 (correlated-molecular structure, Russell et al. 1992)
- 1.186 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
- 1.057 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
- $\ln K_{AW} = 14.233 - 6559.6/(T/K)$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.40 (from Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Dunn III 1972)

- 1.37, 1.38; 1.34 (calculated-fragment const.; calculated- π constant, Rekker 1977)
 1.44, 1.48 (HPLC-RV/RT correlation, Yonezawa & Urushigawa 1979)
 1.53 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 1.33 (HPLC-RT correlation, D'Amboise & Hanai 1982)
 1.56 (shake flask, Log P Database, Hansch & Leo 1987)
 1.49 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 1.53 (generator column-GC, Schantz & Martire 1987)
 1.55 (calculated from measured γ , Schantz & Martire 1987)
 1.51 (recommended value, Sangster 1989, 1993)
 1.41 (shake flask-GC, Fujiwara et al. 1991)
 1.56 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 4.69 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

- 0.241 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

- 0.93 (calculated-MCI χ , Gerstl & Helling 1987)
 0.70 (soil, quoted exptl., Meylan et al. 1992)
 0.65 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 0.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate of $6.92 \times 10^{-5} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate of $(50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^\circ\text{C}$ (Gückel et al. 1973).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH}(\text{exptl}) = 1.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k = 6.50 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with hydroxyl radical in aqueous solution at 298 K (flash photolysis-resonance fluorescence, Wallington & Kurylo 1987)

$k_{OH} = 1.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 10.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (review, Atkinson 1989)

$k_{OH} = (12.0 \pm 1.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (10.5 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.9.1

Reported aqueous solubilities of 1-pentanol at various temperatures

Ginnings & Baum 1937		von Erichsen 1952		Barton 1984		Stephenson et al. 1984	
volumetric method		synthetic method		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	23600	0	30500	0	31000	0	23100
25	21900	10	27000	10	27000	10.2	25900
30	20300	20	23500	20	23100	20.2	22500
		30	21000	25	22000	30.6	20200
		40	19000	30	20400	40.2	18700
		50	18000	40	20000	50.0	18300
		60	18000	50	18000	60.3	18300
		70	18500	60	18000	70.0	19500
		80	19000	70	19000	80.0	19900
		90	20000	80	19000	90.7	22100
		100	22500	90	20000		
		110	26000	100	23000		
		120	30000	110	26000		
		130	35500	120	30000		
		140	43000	130	36000		
		150	53500	140	43000		
		160	69000	150	54000		
		170	95500	160	69000		
		180	175000	170	96000		
				180	175000		

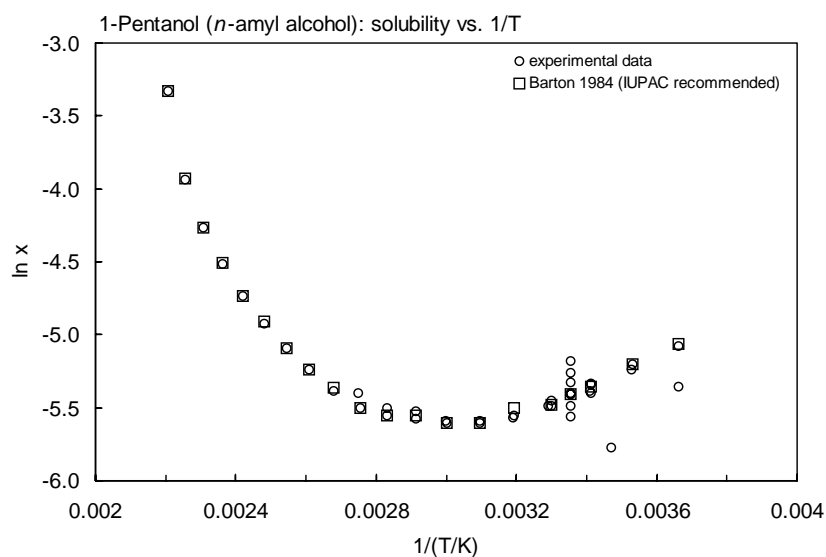
FIGURE 11.1.1.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-pentanol.

TABLE 11.1.1.9.2

Reported vapor pressures of 1-pentanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Butler et al. 1935	Stull 1947	Kemme & Kreps 1969	Ambrose & Sprake 1970				
isoteniscope method	summary of literature data	differential thermal analysis	comparative ebulliometry				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	333.3	13.6	133.3	33.9	573.3	74.763	7175
60.12	3468	34.7	666.6	45.6	1267	83.542	11204
70.3	6153	44.9	1333	52.6	2027	87.571	13615
80.59	10364	55.8	2666	56.7	2640	90.768	15825
90.84	16772	68.0	5333	63.6	3920	95.514	19660
101.17	26398	75.5	7999	69.3	5426	101.629	25714
110.2	38250	85.8	13332	74.9	7306	106.362	31393
120.56	56542	102.0	26664	83.1	11026	110.658	37413
130.89	81580	119.8	53329	90.7	15879	115.564	45399
		137.8	101325	102.4	26664	119.681	53129
bp/°C	137.75			112.3	40263	124.099	62576
D ²⁵	0.8125	mp/°C	-	125.8	66941	128.665	73706
				138.0	102045	133.309	86610
eq. 4	P/mmHg					136.688	97054
A	46.4925			Antoine eq.		138.514	103110
B	4580			eq. 2	P/mmHg	142.435	117105
C	11.42			A	7.55787	146.598	133550
				B	1492.549	151.332	154379
				C	181.529	155.977	177156
$\Delta H_v/(\text{kJ mol}^{-1}) = 56.90$ at 25°C							
				Antoine eq. for full range			
				eq. 3 P/mmHg			
				A 6.30306			
				B 1286.333			
				C 111.843			
				Data also fitted to Cragoe equation, see ref.			

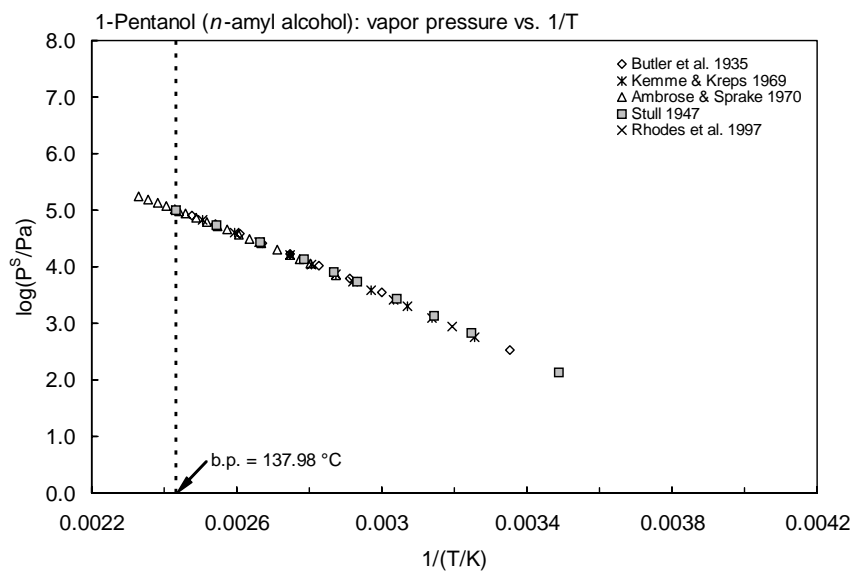
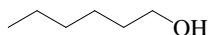


FIGURE 11.1.1.9.2 Logarithm of vapor pressure versus reciprocal temperature for 1-pentanol.

11.1.1.10 1-Hexanol



Common Name: 1-Hexanol

Synonym: amylcarbinol, 1-hexanol, *n*-hexyl alcohol

Chemical Name: *n*-hexyl alcohol, 1-hexanol

CAS Registry No: 111-27-3

Molecular Formula: $C_6H_{14}O$, $CH_3CH_2CH_2CH_2CH_2CH_2OH$

Molecular Weight: 102.174

Melting Point ($^{\circ}C$):

−47.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

157.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8136 (Weast 1982–83)

0.81875, 0.81534 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

126.0 (calculated-density, Lande & Banerjee 1981)

148.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.40 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5000* ($20^{\circ}C$, shake flask-turbidity, measured range 0 – $110^{\circ}C$, Fühner 1924)

6240 (shake flask-interferometer, Butler et al. 1933)

5025 ($20^{\circ}C$, shake flask-turbidity, Laddha & Smith 1948)

6400* ($20^{\circ}C$, synthetic method, measured range 0 – $220^{\circ}C$, von Erichsen 1952)

6000 (shake flask-titration, Crittenden & Hixon 1954)

6300 (estimated, McGowan 1954)

6000 (surface tension, Kinoshita et al. 1958)

5838* (shake flask-refractive index, measured range 5.5 – $33.6^{\circ}C$, Hill & White 1974)

3590 (shake flask-GC, Korenman et al. 1974)

4230 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

6000* (recommended best value, IUPAC Solubility Series, temp range 0 – $220^{\circ}C$, Barton 1984)

6660* ($20^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.3^{\circ}C$, Stephenson et al. 1984)

5354 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

95.86* ($24.98^{\circ}C$, extrapolated-modified isoteniscope data, measured range 60.11 – $152.77^{\circ}C$, Butler et al. 1935)

$\log(P/mmHg) = 51.0030 - 5068/(T/K) - 13.80 \cdot \log(T/K)$, temp range 60 – $152^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

151.1* (interpolated-regression of tabulated data, temp range 24.4 – $157^{\circ}C$, Stull 1947)

88.25 (extrapolated, ebulliometry, measured range 52 – $157^{\circ}C$, Kemme & Kreps 1969)

760* ($52.2^{\circ}C$, ebulliometry-differential thermal analysis, measured range 52.3 – $157.3^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 7.28781 - 1422.031/(t/^{\circ}C + 165.444)$; temp range 52 – $157^{\circ}C$ or pressure range 5.7 – $757.3\ mmHg$ (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

$\log(P/mmHg) = [-0.2185 \times 12708.5/(T/K)] + 9.367617$; temp range 24.4 – $157^{\circ}C$ (Antoine eq., Weast 1972–73)

- 130.6 (20°C, Verschueren 1983)
 79.65, 79.7 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.20107 - 1305.63/(153.901 + t/^{\circ}\text{C})$; temp range 52.2–157.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.26314 - 1334.63/(156.297 + t/^{\circ}\text{C})$; temp range 60.11–152.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 55.5 (extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
 52.9, 254, 888 (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)
 109.5 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.86045 - 1707.26/(196.66 + t/^{\circ}\text{C})$; temp range 35–157°C (Antoine eq., Dean 1985, 1992)
 110 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.41271 - 1422.031/(t/^{\circ}\text{C} + 165.444)$; temp range not specified (Riddick et al. 1986)
 111 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.41271 - 1422.031/(-107.706 + T/\text{K})$; temp range 325–431 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 10.60355 - 3986.406/(46.713 + T/\text{K})$; temp range 298–343 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 53.9686 - 4.9501 \times 10^3/(T/\text{K}) - 15.199 \cdot \log(T/\text{K}) - 6.6922 \times 10^{-10} \cdot (T/\text{K}) + 2.3647 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 229–611 K (vapor pressure eq., Yaws 1994)
 113* (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)
 $\ln(P/\text{kPa}) = 8.472727 - 1275.055/(T/\text{K} - 178.568)$; temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 1.562 (measured partial pressure/mole fraction x at dilute aqueous solution, Butler et al. 1935)
 1.735 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 1.562 (exptl., Hine & Mookerjee 1975)
 1.88, 2.367 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.46 (limiting activity coefficient by headspace-GC., Abraham et al. 1987)
 1.60 (calculated-MCI χ , Nirmalakhandan & Speece 1988b)
 1.896 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 1.56 (limiting activity coefficient by headspace-GC., Li & Carr 1993)
 1.016 (wetted-wall column-GC, Altschuh et al. 1999)
 2.60 (extrapolated-headspace GC data, measured range 40–90°C, Gupta et al. 2000)
 $\ln K_{\text{AW}} = 11.705 - 5538.7/(T/\text{K})$; temp range 40–90°C (van't Hoff eq., headspace GC, Gupta et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 2.03 (shake flask-GC, Hansch & Anderson 1967; Leo et al. 1971; Hansch & Dunn III 1972)
 1.99 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
 2.03 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 1.86 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 2.03 (HPLC- k' correlation, Funasaki et al. 1986)
 2.04 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 2.03 (generator column-GC, Schantz & Martire 1987)
 2.05 (calculated from measured γ , Schantz & Martire 1987)
 1.50 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 2.03 (recommended, Sangster 1989, 1993)
 2.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 5.18 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.711 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC} :

1.01	(soil, quoted exptl., Meylan et al. 1992)
0.92	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.01	(calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate of $1.85 \times 10^{-5} \text{ mol}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$ was determined by gravimetric method with an air flow rate of $(50 \pm 1) \text{ L}\cdot\text{h}^{-1}$ at $(20 \pm 0.1)^\circ\text{C}$ (Gückel et al. 1973).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH}(\text{exptl}) = (12.4 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 10.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{OH}(\text{exptl}) = 1.24 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, and $k(\text{soln}) = 1.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 12.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH} = (12.2 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by pulse radiolysis-UV spectroscopy; $k_{OH} = (12.9 \pm 1.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by relative rate method, at $298 \pm 2 \text{ K}$ (Nelson et al. 1990)

$k_{OH}(\text{calc}) = 10.48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water:

Groundwater:

Sediment:

Soil:

Biota

TABLE 11.1.1.10.1

Reported aqueous solubilities of 1-hexanol at various temperatures

1.

Fühner 1924		von Erichsen 1952		Hill & White 1974		Barton 1984	
synthetic method		synthetic method		shake flask-interferometry		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	7800	0	8100	5.51	7879	0	7900
10	6700	10	7000	6.85	7655	10	6900
20	5900	20	6400	8.15	7375	20	6200
30	5450	30	5900	11.0	7061	25	6000
40	5200	40	5400	12.94	6820	30	5700
50	5150	50	5000	14.68	6651	40	5300
60	5300	60	5200	17.04	6427	50	5100
70	5650	70	5600	20.71	6124	60	5200
80	6200	80	6100	22.99	5894	70	5600

(Continued)

TABLE 11.1.1.10.1 (Continued)

Fühner 1924		von Erichsen 1952		Hill & White 1974		Barton 1984	
synthetic method		synthetic method		shake flask-interferometry		IUPAC recommended	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
90	6800	90	6900	25.01	5838	80	6200
100	7850	100	8000	26.99	5764	90	6900
110	8900	110	9100	28.94	5702	100	7900
		120	10400	30.92	5639	110	9000
		130	11900	33.59	5560	120	10000
		140	13700			130	12000
		150	16300			140	14000
		160	20500			150	16000
		170	27000			160	21000
		180	36100			170	27000
		190	48700			180	36000
		200	67500			190	49000
		210	97000			200	68000
		220	163000			210	97000
						220	163000

2.

Stephenson et al. 1984

shake flask-GC/TC	
t/°C	S/g·m ⁻³
0	9640
10.2	7590
20.0	6660
29.7	5580
39.8	5140
50.0	4970
60.0	5180
70.3	5770
80.3	6250
90.3	6380

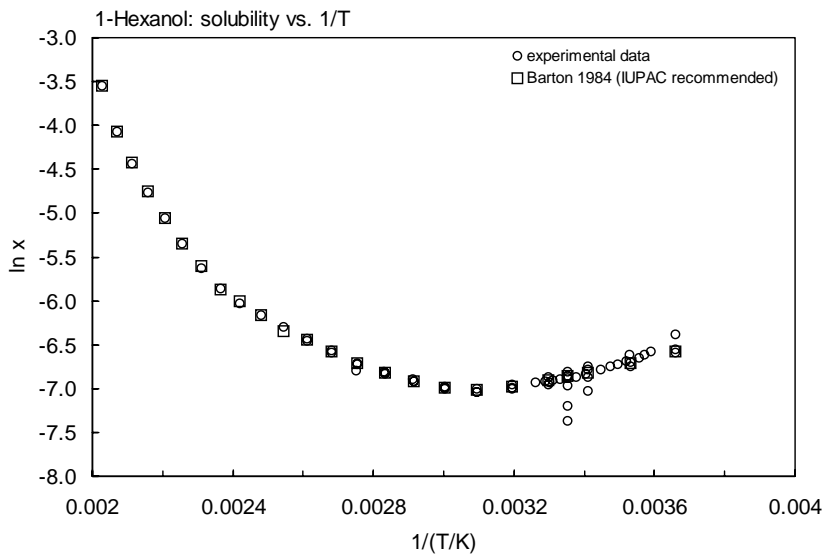


FIGURE 11.1.1.10.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-hexanol.

TABLE 11.1.1.10.2
Reported vapor pressures of 1-hexanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)	ln P = A –B/(C + T/K)		(3a)		
log P = A – B/(T/K) – C·log (T/K)		(4)					
Butler et al. 1935		Stull 1947		Kemme & Kreps 1969		Garriga et al. 1996	
static method-isoteniscope		summary of literature data		differential thermal analysis		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	95.86	24.4	133.3	52.2	760.0	5	13
60.11	1300	47.2	666.6	60.4	1293	10	24
70.29	2365	58.2	1333	67.4	2040	15	45
80.58	4213	70.3	2666	72.6	2733	20	68
90.83	7275	83.7	5333	79.2	3973	25	113
101.16	12000	92.0	7999	85.0	5436	30	169
110.19	18012	102.8	13332	91.1	7373	35	251
120.55	27624	119.6	26664	98.7	10666	40	369
130.88	41303	138.0	53329	107.6	16105	45	517
141.67	60901	157.0	101325	119.7	26798	50	713
152.77	87966			130.1	40237		
		mp/°C	–51.6	144.5	66661	Antoine eq.	
bp/°C	155.7			157.3	100965	eq. 3a	P/kPa
D ²⁵	0.8183					A	8.472727
				Antoine eq.		B	1275.055
eq. 4	P/mmHg			eq. 2	P/mmHg	C	–178.875
A	51.003			A	7.28781		
B	5068			B	1422.031		
C	13.80			C	165.444		
ΔH _v /(kJ mol ^{–1}) = 62.84							
at 25°C							

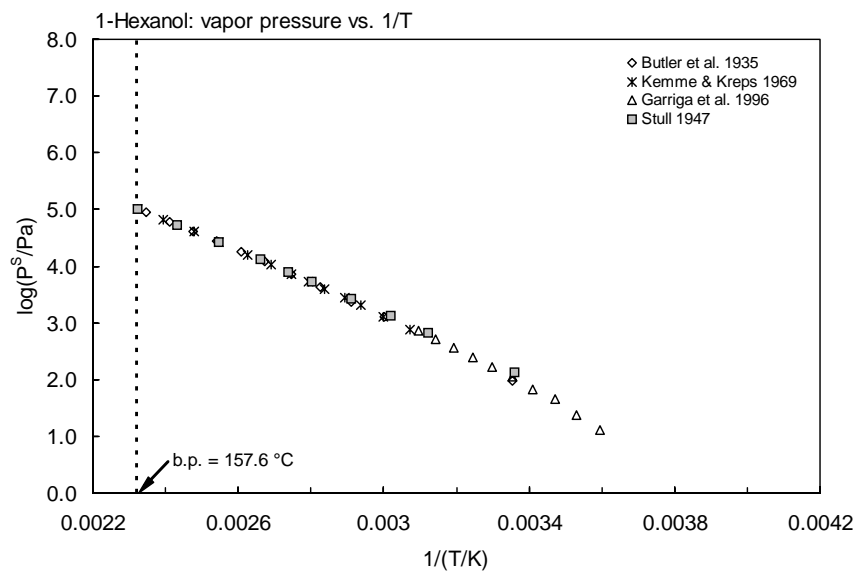
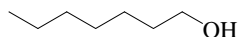


FIGURE 11.1.10.2 Logarithm of vapor pressure versus reciprocal temperature for 1-hexanol.

11.1.1.11 1-Heptanol



Common Name: 1-Heptanol

Synonym: 1-heptanol, *n*-heptyl alcohol

Chemical Name: *n*-heptyl alcohol, 1-heptanol

CAS Registry No: 111-70-6

Molecular Formula: $C_7H_{16}O$, $CH_3(CH_2)_6OH$

Molecular Weight: 116.201

Melting Point ($^{\circ}C$):

−33.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

176.45 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.82053 ($25^{\circ}C$, Butler et al. 1935)

0.8219 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

142.0 (calculated-density, Lande & Banerjee 1981)

170.2 (calculated- Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

930* ($18^{\circ}C$, shake flask-turbidity, measured range 70 – $130^{\circ}C$, Fühner 1924)

1804 (shake flask-interferometer, Butler et al. 1933)

1720 ($20^{\circ}C$, shake flask-titration, Addison 1943)

3288 (shake flask-centrifuge, Booth & Everson 1948)

1200 (shake flask-turbidimetric method, Harkins & Oppenheimer 1949)

2000* ($20^{\circ}C$, synthetic method, measured range 0 – $245^{\circ}C$, von Erichsen 1952)

1800 (estimated, McGowan 1954)

1700 (surface tension, Kinoshita et al. 1958)

1500* ($20^{\circ}C$, surface tension, 15 – $60^{\circ}C$, measured range Vochten & Petre 1973)

1676* (shake flask-interferometric method, measured range 6 – $34.9^{\circ}C$, Hill & White 1974)

1313 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

1740* (recommended best value, IUPAC Solubility Data Series, temp range 0 – $240^{\circ}C$, Barton 1984)

1840* ($20.2^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.5^{\circ}C$, Stephenson et al. 1984)

1510 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29.86* (extrapolated, modified isoteniscope method, measured range 60 – $110^{\circ}C$, Butler et al. 1935)

$\log(P/mmHg) = 55.1972 - 5580/(T/K) - 15.41 \cdot \log(T/K)$; temp range 60 – $152^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

44.04* (extrapolated-regression of tabulated data, temp range 42.4 – $175.8^{\circ}C$, Stull 1947)

22.2 (extrapolated-Antoine eq., ebulliometry, Kemme & Kreps 1969)

626.6* ($63.5^{\circ}C$, ebulliometry-differential thermal analysis, measured range 63.6 – $176.4^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 6.85450 - 1266.783/(139.663 + t/^{\circ}C)$; temp range 63.6 – $176.4^{\circ}C$, or pressure range 5.3 – 760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

31.30 (calculated-Antoine eq., Jordan 1970)

$\log(P/mmHg) = [-0.2185 \times 13920.9/(T/K)] + 9.720613$; temp range 42.4 – $175.8^{\circ}C$ (Antoine eq., Weast 1972–73)

- 12.8 (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
- 24.0 (extrapolated-Antoine eq., Boublik et al. 1984)
- $\log(P/\text{kPa}) = 6.10824 - 1323.566/(146.241 + t/^{\circ}\text{C})$; temp range 63.6–176.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log(P/\text{kPa}) = 6.01857 - 1278.78/(146.403 + t/^{\circ}\text{C})$; temp range 60.11–152.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 17.64 (extrapolated-Antoine eq., Dean 1985)
- $\log(P/\text{mmHg}) = 6.64767 - 1140.64/(126.56 + t/^{\circ}\text{C})$; temp range 60–176°C (Antoine eq., Dean 1985, 1992)
- $\log(P_L/\text{kPa}) = 5.9794 - 1256.783/(-133.487 + T/\text{K})$; temp range 336–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.10408 - 1322.62/(-126.87 + T/\text{K})$; temp range 335–450 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P/\text{mmHg}) = -19.9205 - 4.3239 \times 10^3/(T/\text{K}) + 18.794 \cdot \log(T/\text{K}) - 5.0553 \times 10^{-2} \cdot (T/\text{K}) + 2.6161 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 239–632 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

- 1.909 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
- 1.880 (exptl., Hine & Mookerjee 1975)
- 2.656, 3.583 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 2.015 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 1.176 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
- 5.55 (calculated-molecular structure, Russell et al. 1992)
- 5.62 (gas stripping-GC, Shiu & Mackay 1997)
- 1.165 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.53 (Hansch & Dunn III 1972)
- 2.41 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
- 2.57 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
- 2.39 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
- 2.60 (HPLC- k' correlation, Funasaki et al. 1986)
- 2.65 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
- 2.57 (shake flask, Log P Database, Hansch & Leo 1987)
- 2.57 (generator column-GC, Schantz & Martire 1987)
- 2.57 (calculated-activity coeff. γ , Schantz & Martire 1987)
- 1.83 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
- 2.62 (recommended, Sangster 1989, 1993)
- 2.72 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

- 1.09 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, $\log K_{oc}$:

- 1.48 (calculated-MCI χ , Gerstl & Helling 1987)
- 1.14 (soil, quoted exptl., Meylan et al. 1992)
- 1.19 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.14 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate of $6.804 \times 10^{-6} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate of $(50 \pm 1) \text{ L h}^{-1}$ at 20°C (Gückel et al. 1973).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical in air (Darnall et al. 1976)

$k_{\text{OH}}(\text{exptl}) = (13.6 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 10.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{\text{OH}}(\text{exptl}) = 1.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k(\text{soln}) = 1.20 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the s reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}} = (13.7 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 2 K (relative rate method, Nelson et al. 1990)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical in air (Darnall et al. 1976).

Surface water:

Sediment:

Soil:

Biota:

TABLE 11.1.1.11.1

Reported aqueous solubilities of 1-heptanol at various temperatures

1.

Fühner 1924		von Erichsen 1952		Vochten & Petre 1973		Hill & White 1974	
synthetic method		synthetic method		surface tension measurement		shake flask-interferometer	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
70	1250	0	3400	15	2000	6.0	2204
80	1700	10	2600	20	1500	10.2	2020
90	2250	20	2000	30	1500	10.54	1998
100	2800	30	1600	40	1300	15.08	1868
110	3350	40	1300	50	1400	17.94	1794
120	4300	50	1100	60	1500	20.03	1750
130	5150	60	1100			21.9	1685
		70	1500			24.99	1676
		80	1900			25.07	1665
		90	2300			26.04	1652
		100	2900			28.02	1639
		110	3500			30.14	1623
		120	4300			30.16	1625
		130	5300			32.9	1610
		140	6500			34.9	1605
		150	8000				
		160	9800				
		170	12300				
		180	16000				
		190	20800				
		200	25400				
		210	34800				

(Continued)

TABLE 11.1.1.11.1 (Continued)

Fühner 1924		von Erichsen 1952		Vochten & Petre 1973		Hill & White 1974	
synthetic method		synthetic method		surface tension measurement		shake flask-interferometer	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
		220	46800				
		230	67000				
		240	101000				
		245	139600				

2.

Barton 1984				Stephenson et al. 1984	
IUPAC recommended				shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
0	3400	120	4300	0	2360
10	2500	130	5200	10.5	2530
20	1700	140	6500	20.2	1840
25	1740	150	8000	30.6	1540
30	1600	160	10000	39.8	1660
40	1300	170	12000	50.1	1620
50	1200	180	16000	60.0	1780
60	1300	190	21000	70.1	2040
70	1400	200	26000	80.1	2170
80	1800	210	35000	90.5	2430
90	2300	220	47000		
100	2900	230	67000		
110	3400	240	101000		

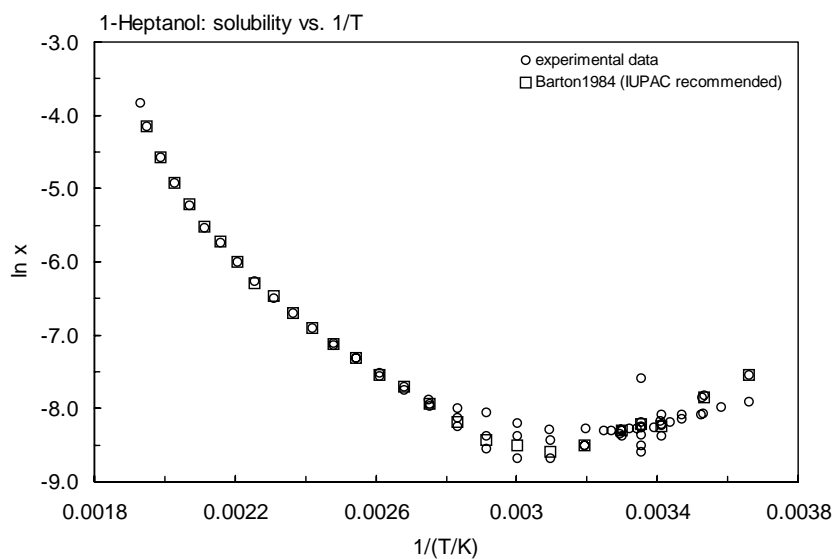
FIGURE 11.1.1.11.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-heptanol.

TABLE 11.1.1.11.2
Reported vapor pressures of 1-heptanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Butler et al. 1935		Stull 1947		Kemme & Kreps 1969	
isoteniscopes method		summary of literature data		differential thermal analysis	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	29.86	42.4	133.3	63.6	626.6
68.11	505	64.3	666.6	76.1	1453
70.29	997	74.7	1333	81.5	2000
80.58	1913	85.8	2666	87.6	2813
90.83	3430	99.8	5333	94.3	4026
101.16	5882	108.0	7999	99.9	5360
110.10	9061	119.5	13332	106.4	7399
120.55	14292	136.6	26664	114.5	10732
130.88	21811	155.6	53329	124.1	16319
141.67	32864	175.8	101325	136.5	26798
152.77	48596			147.8	40463
		mp/°C	34.6	162.8	66794
bp/°C	175.6			178.4	101432
D ²⁵	0.8205				
		Antoine eq.			
eq. 4	P/mmHg			eq. 2	P/mmHg
A	56.1972			A	6.85450
B	5580			B	1256.783
C	15.41			C	139.663
$\Delta H_v/(\text{kJ mol}^{-1}) = 68.66$					
at 25°C					

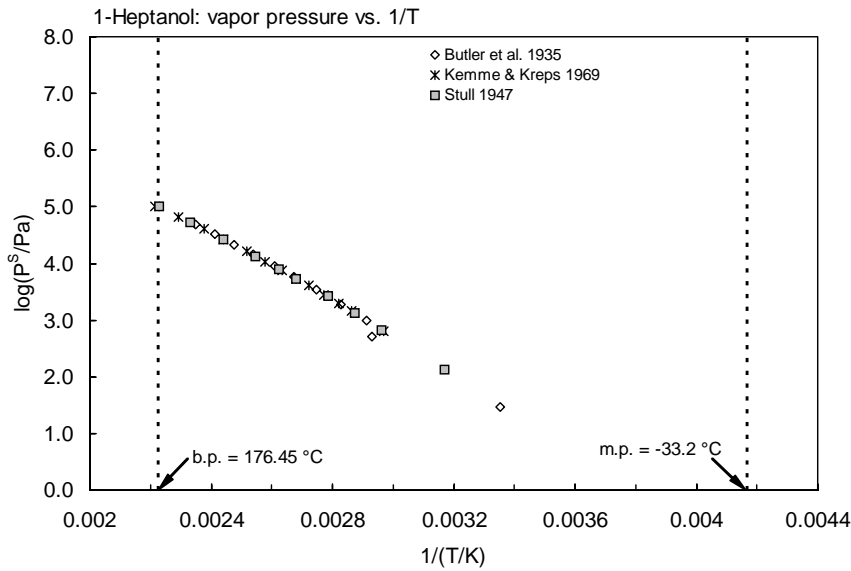
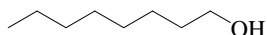


FIGURE 11.1.1.11.2 Logarithm of vapor pressure versus reciprocal temperature for 1-heptanol.

11.1.1.12 1-Octanol (*n*-Octyl alcohol)

Common Name: 1-Octanol

Synonym: 1-octanol, *n*-octyl alcohol, capryl alcohol, heptylcarbinol

Chemical Name: *n*-octyl alcohol, 1-octanol

CAS Registry No: 111-87-5

Molecular Formula: $C_8H_{18}O$, $CH_3(CH_2)_7OH$

Molecular Weight: 130.228

Melting Point ($^{\circ}C$):

−14.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

195.15 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.827 (Weast 1982–83)

0.82499, 0.82157 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

158.0 (calculated-density, Rohrschneider 1973; Lande & Banerjee 1981)

192.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

42.3 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

56 (estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

586 (shake flask-interferometer, Butler et al. 1933)

760 ($30^{\circ}C$, shake flask-titration, Sobotka & Glick 1934.)

420 ($20^{\circ}C$, shake flask-surface tension, Addison 1945)

590 (shake flask-turbidimeter, McBain & Richard 1946)

500 (shake flask-titration, Crittenden & Hixon 1954)

582 (estimated, McGowan 1954)

490 (shake flask-surface tension, Kinoshita et al. 1958)

495 (shake flask-turbidity, Shinoda et al. 1959)

1000 ($30^{\circ}C$, shake flask-turbidimeter, Rao et al. 1961)

330 (calculated- K_{OW} , Hansch et al. 1968)

530 ($15^{\circ}C$, shake flask-surface tension, Vochten & Petre 1973)

600, 600 (40 , $60^{\circ}C$, shake flask-titration, Lavrova & Lesteva 1976)

10000, 5000 (95 , $115^{\circ}C$, shake flask-polythermic method, Zhuravleva et al. 1977)

540* (recommended best value, IUPAC Solubility Data Series, temp range 15 – $115^{\circ}C$, Barton 1984)

490* ($20.5^{\circ}C$, shake flask-GC/TC, measured range 20.5 – $90.3^{\circ}C$, Stephenson et al. 1984)

517 (shake flask-GC, Li et al. 1992)

417 (shake flask-GC, Li & Andren 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11.06* ($25^{\circ}C$, extrapolated-modified isoteniscope data, measured range 60.12 – $110^{\circ}C$, Butler et al. 1935)

$\log (P/mmHg) = 40.2105 - 4100/(T/K) - 10.35 \cdot \log (T/K)$; temp range 20 – $110^{\circ}C$ (isoteniscope measurements, Butler et al. 1935)

18.8* (extrapolated-regression of tabulated data, temp range 54 – $195.2^{\circ}C$, Stull 1947)

$\log (P/mmHg) = 8.29442 - 2302.3/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

7604* ($121.99^{\circ}C$, ebulliometry, measured range 121.99 – $195.28^{\circ}C$, Dreisbach & Shrader 1949)

- 5.28 (extrapolated-Antoine eq., ebulliometry- DTA, Kemme & Kreps 1969)
- 706.6* (78.9°C, ebulliometry-differential thermal analysis, measured range 78.9–195.3°C, Kemme & Kreps 1969)
- $\log (P/\text{mmHg}) = 6.62354 - 1196.639/(124.107 + t/^{\circ}\text{C})$; temp range 78.9–195.3°C, or pressure range 5.3–760 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
- 10* (comparative ebulliometry, measured range 113.274–206.123 K, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 5.79413 - 1434.755/(T/\text{K} - 149.407)$; restricted temp range 113.274–151.974°C, (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- $\log (P/\text{Pa}) = 5.88511 - 1264.322/(T/\text{K} - 142.420)$; temp range 113.274–206.123°C (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- 142* (54.88°C, comparative ebulliometry, measured range 328.03–386.96 K, data fitted to Chebyshev polynomial, Ambrose et al. 1974)
- 2.78 (20°C, extrapolated from Antoine eq. of Kemme & Kreps 1969, Gückel et al. 1982)
- 4.07, 32.3, 177 (20, 40, 60°C, evaporation rate-gravimetric method, Gückel et al. 1982)
- $\log (P/\text{mmHg}) = [-0.2185 \times 14262.4/(T/\text{K})] + 9.601156$; temp range: 54–195°C, (Antoine eq., Weast 1972–73)
- 10.06, 6.89, 5.74, 9.95 (extrapolated-Antoine eq., Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.80512 - 1752.302/(174.07 + t/^{\circ}\text{C})$; temp range 54.88–113.9°C (Antoine eq. from reported exptl. data of Ambrose et al. 1974, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 5.98227 - 1322.952/(137.413 + t/^{\circ}\text{C})$; temp range 79.9–195.4°C (Antoine eq. from reported exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 5.87970 - 1260.554/(130.23 + t/^{\circ}\text{C})$; temp range 113.3–206.1°C (Antoine eq. from reported exptl. data of Ambrose & Sprake 1970, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.00162 - 1356.232/(144.452 + t/^{\circ}\text{C})$; temp range 229.05–250.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 13.43 (calculated-Antoine eq., Dean 1985)
- $\log (P/\text{mmHg}) = 12.0701 - 4506.8/(319.9 + t/^{\circ}\text{C})$; temp range 0–80°C (Antoine eq., Dean 1985, 1992)
- $\log (P/\text{mmHg}) = 6.83790 - 1310.62/(136.05 + t/^{\circ}\text{C})$; temp range 70–195°C (Antoine eq., Dean 1985, 1992)
- 14.5 (static measurement, Berti et al. 1986)
- 10.0 (Riddick et al. 1986)
- $\log (P/\text{kPa}) = 5.88511 - 1264.322/(t/^{\circ}\text{C} + 130.73)$; temp range not specified (Riddick et al. 1986)
- 13.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.90052 - 1273.291/(-141.417 + T/\text{K})$; temp range 386–480 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.342 - 3343/(T/\text{K})$; temp range 267–282 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 18.014 - 5507/(T/\text{K})$; temp range 238–251 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.7934 - 1208.201/(-149.366 + T/\text{K})$; temp range 430–474 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.39406 - 1540.599/(-114.618 + T/\text{K})$; temp range 328–400 K (Antoine eq.-V, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 5.90632 - 1276.86/(-140.996 + T/\text{K})$; temp range 397–479 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
- 10.58 (Daubert & Danner 1989; quoted, Howard 1993)
- $\log (P/\text{mmHg}) = -26.3876 - 4.2263 \times 10^3/(T/\text{K}) + 21.093 \cdot \log(T/\text{K}) - 5.0048 \times 10^{-2} \cdot (T/\text{K}) + 2.4611 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 258–653 K (vapor pressure eq., Yaws 1994)
- 8.0* (static method-manometry, measured range 278.15–323.15 K, Garriga et al. 1996)
- $\ln (P/\text{kPa}) = 13.058110 - 2443.493/(T/\text{K} - 162.071)$; temp range 278.15–323.15 K (Antoine eq., static method-manometry, Garriga et al. 1996)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 2.454 (measured partial pressure/mole fraction x at dilute concn, Butler et al. 1935)
- 2.479 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
- 2.422 (exptl., Hine & Mookerjee 1975)
- 3.344, 6.085 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 2.537 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

- 1.609 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 1.537 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, log K_{OW} :

- 3.15 (shake flask-CR, Collander 1951)
 2.84 (calculated- π constant, Hansch et al. 1968)
 3.03 (Hansch & Dunn III 1972)
 2.95, 2.97; 2.84 (calculated-f const.; calculated- π constant, Rekker 1977)
 2.97 (HPLC- k' correlation, Könemann et al. 1979)
 2.80 (HPLC-RV correlation, Yonezawa & Urushigawa 1979)
 2.92 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 3.16 (shake flask-GC, Platford 1983)
 2.97 (Hansch & Leo 1985)
 3.27 (shake flask-GC at pH 7, Riebesehl & Tomlinson 1986)
 2.14 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 3.07 (recommended, Sangster 1989, 1993)
 3.00 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

- 6.03 (calculated-measured γ^∞ in pure octanol and vapor pressure P, Abraham et al. 2001)

Bioconcentration Factor, log BCF:

- 0.307 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
 0.097 (calculated-S, Lyman et al. 1982; quoted, Howard 1993)
 1.651 (calculated as per Mackay 1982, Schultz et al. 1990)

Sorption Partition Coefficient, log K_{OC} :

- 2.99 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)
 2.14 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1993)
 1.56, 1.76 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
 1.56 (soil, quoted exptl., Meylan et al. 1992)
 1.45 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 1.56 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate $k = 1.752 \times 10^{-6} \text{ mol}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$ was determined by gravimetric method with an air flow rate $k = (50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^\circ\text{C}$ (Gückel et al. 1973);

$t_{1/2} \sim 1.8 \text{ d}$ from a model river of 1-m deep flowing at 1 m/s with a wind speed of 3 m/s, based on calculated Henry's law constant (Lyman et al. 1982; quoted, Howard 1993);

$t_{1/2} \sim 8.2 \text{ d}$ from a model pond with the consideration of adsorption (USEPA 1987; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k, for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation half-life of 0.24–2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k \leq 0.8 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (13.6 \pm 1.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Wallington et al. 1988a; Atkinson 1989)

$k_{OH} = (14.4 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (relative rate method, Nelson et al. 1990)

$k_{OH}(\text{calc}) = 11.67 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 1.3$ d in air, based on measured rate constant $k = 1.195 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radical of $5 \times 10^5 \text{ cm}^{-3}$ at 25°C in air (Atkinson 1987; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.12.1

Reported aqueous solubilities of 1-octanol at various temperatures

Barton 1984		Stephenson et al. 1984	
tentative or recommended		shake flask-GC/TC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
15	530	20.5	490
20	420	30.6	640
25	540	40.1	650
30	760	50.0	1050
40	600	60.3	880
60	600	70.3	770
95	1000	80.1	870
115	500	90.3	860
25	540*		
30	900*		

*"best" values

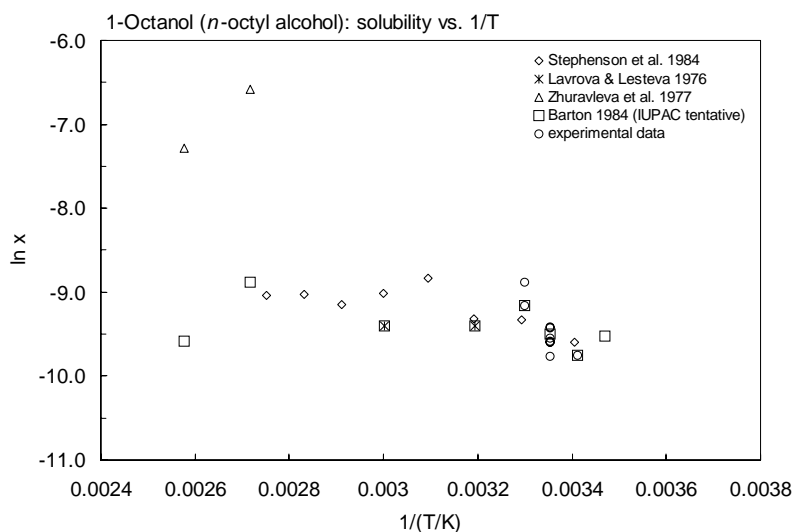
FIGURE 11.1.1.12.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 1-octanol.

TABLE 11.1.1.12.2

Reported vapor pressures of 1-octanol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & \ln P = A - B/(C + T/K) & (3a) \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Butler et al. 1935		Stull 1947		Dreisbach & Shrader 1949		Kemme & Kreps 1969	
isoteniscope method		summary of literature data		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.98	11.066	54.0	133.3	121.99	7604	78.9	706.6
60.12	220.0	76.5	666.6	125.42	8851	88.8	1360
70.3	441.3	88.3	1333	140.37	16500	95.4	2000
80.59	890.6	101.0	2666	166.09	42066	101.5	2800
90.84	1589	115.2	5333	181.17	67661	108.4	4000
101.17	2868	123.8	7999	195.28	101325	114.0	5266
110.2	4456	135.2	13332			120.9	7253
120.56	7202	152.0	26664			131.2	11386
130.89	11390	173.8	53329			140.2	16505
141.68	17683	195.2	101325			166.1	42063
152.78	26858					181.2	67674
		mp/°C	-15.4			195.3	101325
bp/°C	194.5						
D ²⁵	0.8232					Antoine eq.	
						eq. 2	P/mmHg
eq. 4	P/mmHg					A	6.62354
A	65.2106					B	1196.639
B	6190					C	124.107
C	18.40						
$\Delta H_v(\text{kJ mol}^{-1}) = 72.93$							
at 25°C							

2.

Ambrose & Sprake 1970		Ambrose et al. 1974		Garriga et al. 1996	
comparative ebulliometry		comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
113.274	5065	54.88	142	5	< 2
117.718	6261	64.11	281	10	< 2
122.526	7810	70.44	431	15	< 2
127.503	9742	73.91	544	20	3
133.164	12400	77.69	700	25	8
139.162	15845	79.86	803	30	15
147.224	21679	82.36	938	35	25
151.974	25859	84.65	1078	40	45
157.372	31373	87.26	1259	45	77
161.868	36654	89.24	1415	50	116
167.897	44832	91.26	1591		
173.981	54475	95.52	2022	Antoine eq.	

TABLE 11.1.1.12.2 (Continued)

Ambrose & Sprake 1970		Ambrose et al. 1974		Garriga et al. 1996	
comparative ebulliometry		comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
179.523	64637	101.66	2817	eq. 3a	P/Pa
184.300	74519	105.12	5376	A	13.058110
190.026	87866	109.57	4226	B	2443.493
195.114	101222	113.81	5236	C	−162.071
195.504	102265	data fitted to Chebyshev polynomial, see ref.			
201.198	119164				
206.123	135431				
Antoine eq. for full range					
eq. 3	P/Pa				
A	5.88511				
B	1264.322				
C	−142.420				
Data also fitted to Cragoe equation, see ref.					

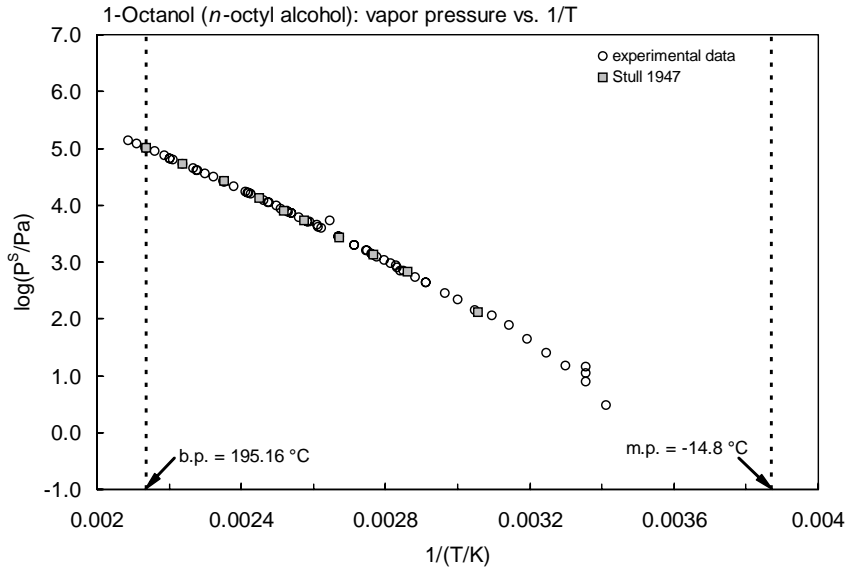
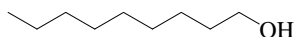


FIGURE 11.1.1.12.2 Logarithm of vapor pressure versus reciprocal temperature for 1-octanol.

11.1.1.13 1-Nonanol



Common Name: 1-Nonanol

Synonym: *n*-nonyl alcohol

Chemical Name: 1-nonanol

CAS Registry No: 143-08-8

Molecular Formula: $C_9H_{20}O$, $CH_3(CH_2)_8OH$

Molecular Weight: 144.254

Melting Point ($^{\circ}C$):

−5 (Lide 2003)

Boiling Point ($^{\circ}C$):

213.37 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8273 (Weast 1982–83)

Molar Volume (cm^3/mol):

174.4 ($20^{\circ}C$, Stephenson and Malanowski 1987)

214.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

140 (shake flask-surface tension, Kinoshita et al. 1958)

140 ($15^{\circ}C$, shake flask-surface tension, Vochten and Petre 1973)

130 (recommended-IUPAC Solubility Data Series, Barton 1984)

280* ($20^{\circ}C$, shake flask-GC/TC, measured range 9.8 – $90.5^{\circ}C$, Stephenson & Stuart 1986)

128 ($20^{\circ}C$, shake flask/slow stirring-GC, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and the reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($59.5^{\circ}C$, summary of literature data, temp range 59.5 – $213.5^{\circ}C$, Stull 1947)

746.6* ($91.7^{\circ}C$, ebulliometry-differential thermal analysis, measured range 91.7 – $213.6^{\circ}C$, Kemme & Kreps 1969)

$\log(P/mmHg) = 6.83667 - 1373.417/(133.968 + t/^{\circ}C)$; temp range 91.7 – $213.6^{\circ}C$, or pressure range 5.6 – 757.5 mmHg (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)

$\log(P/mmHg) = [-0.2185 \times 14065.1/(T/K)] + 8.99150$; temp range 69.5 – $231^{\circ}C$ (Antoine eq., Weast 1972–73)

7.466 ($20^{\circ}C$, extrapolated from data of Stull 1947, Gückel et al. 1973)

1.87 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel et al. 1973)

12680* ($152.15^{\circ}C$, ebulliometry, measured range 152 – $221.35^{\circ}C$, Hon et al. 1976)

0.106 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel et al. 1982)

$\log(P_L/kPa) = 5.9049 - 1341.28/(-142.64 + T/K)$; temp range 381 – 495 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.9454 - 1366.566/(-139.73 + T/K)$; temp range 368 – 500 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 103.0308 - 8.1526 \times 10^3/(T/K) - 31.641 \cdot \log(T/K) - 7.230 \times 10^{-10} \cdot (T/K) + 6.0332 \times 10^{-6} \cdot (T/K)^2$; temp range 280 – 690 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.675 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)

- Octanol/Water Partition Coefficient, log K_{OW} :
- 3.77 (generator column-GC, Tewari et al. 1982)
 - 4.26 (shake flask, Log P Database, Hansch & Leo 1987)
 - 4.26 (recommended, Sangster 1993)
 - 4.26 (shake flask, recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF or log K_B :

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 11.1.1.13.1
Reported aqueous solubilities of 1-nonanol at various temperatures
Stephenson & Stuart 1986

shake flask-GC/TC	
t/°C	S/g·m ⁻³
9.8	350
20.0	280
29.6	310
39.6	340
49.8	320
60.1	340
70.5	330
80.2	280
90.5	300

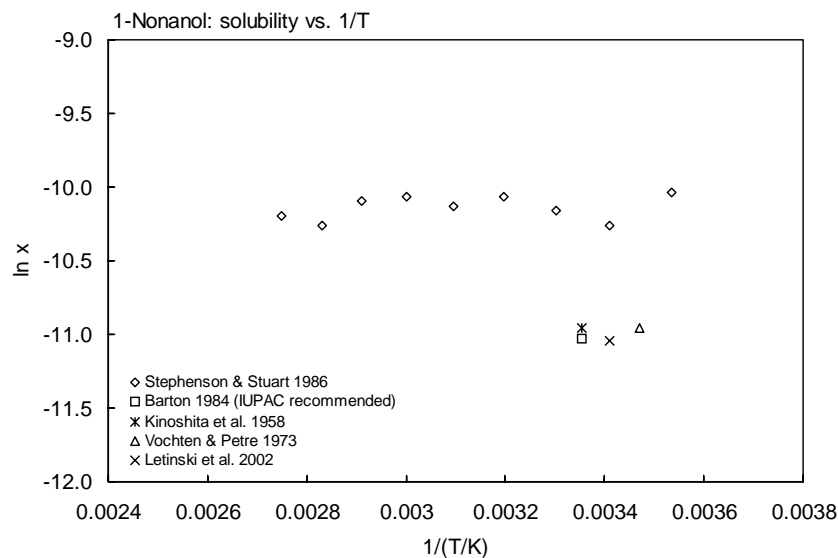


FIGURE 11.1.1.13.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-nonanol.

TABLE 11.1.1.13.2

Reported vapor pressures of 1-nonanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)			
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Kemme & Kreps 1969		Hon et al. 1976	
summary of literature data		differential thermal analysis		ebulliometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
ebulliometry					
59.5	133.1	91.7	746.6	152.15	12680
86.1	666.6	102.1	1400	170.20	25385
99.7	1333	108.9	2040	181.03	37146
113.8	2666	114.4	2706	187.49	46110
129.0	5333	122.4	4026	194.80	58337
139.0	7999	128.8	5413	203.95	77352
151.3	13332	135.8	7399	207.76	86645
170.5	26664	144.7	10719	213.44	101948
192.1	53329	155.0	16092	213.97	103527
213.5	101325	169.0	26851	217.73	115289
		181.0	40317	221.35	127515
mp/ $^{\circ}\text{C}$	-5	198.0	66994		
		213.6	101845	bp/ $^{\circ}\text{C}$	213.17
		Antoine eq.		eq. 2	
		eq. 2		A	
		P/mmHg		B	
		A		C	
		6.83667		7.60022	
		1373.417		1793.77	
		133.968		166.91	

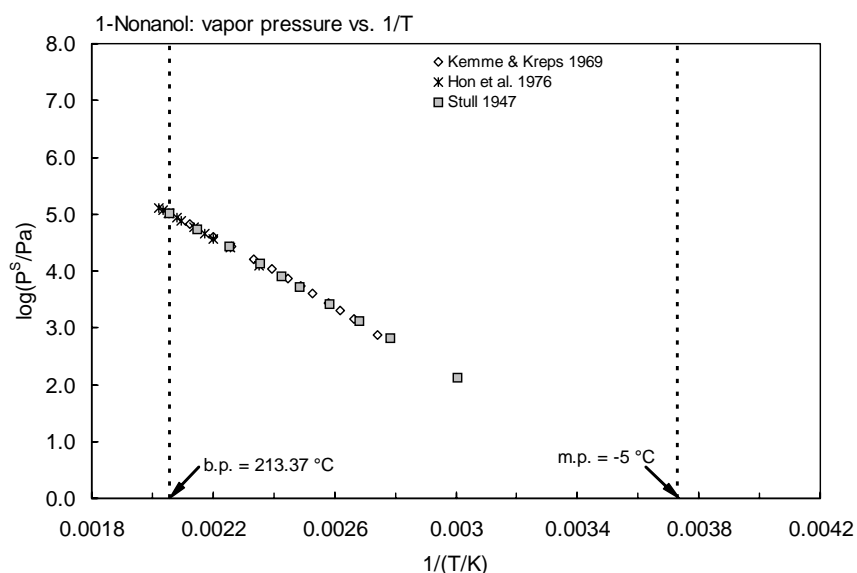
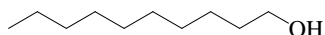


FIGURE 11.1.1.13.2 Logarithm of vapor pressure versus reciprocal temperature for 1-nonanol.

11.1.1.14 1-Decanol



Common Name: 1-Decanol

Synonym: decyl alcohol

Chemical Name: 1-decanol

CAS Registry No: 112-30-1

Molecular Formula: $C_{10}H_{22}O$, $CH_3(CH_2)_8CH_2OH$

Molecular Weight: 158.281

Melting Point ($^{\circ}C$):

6.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

231.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8297 (Weast 1982–83)

Molar Volume (cm^3/mol):

190.8 ($20^{\circ}C$, calculated-density, Stephenson and Malanowski 1987)

236.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

- 50 (shake flask-turbidimetric method, Stearns et al. 1947)
- 36 ($20^{\circ}C$, shake flask-surface tension, Addison and Hutchinson 1949)
- 50 (shake flask-turbidimetric method-photometer, Harkins and Oppenheimer 1949)
- 37 (shake flask-surface tension, Kinoshita et al. 1958)
- 32 ($15^{\circ}C$, shake flask-surface tension, Vochten and Petre 1973)
- 10000, 8000 ($102.5, 120.5^{\circ}C$, polythermic method, Zhuravleva et al. 1977)
- 37* (recommended-IUPAC Solubility Data Series, temp range 15 – $120^{\circ}C$, Barton 1984)
- 210* ($29.6^{\circ}C$, shake flask-GC/TC, measured range 29.6 – $90.4^{\circ}C$, Stephenson 1992)
- 35.9 (dialysis tubing equilibration-GC, Etzweiler et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 133.3* ($69.5^{\circ}C$, summary of literature data, temp range 69.5 – $231.0^{\circ}C$, Stull 1947)
- 747* ($105.0^{\circ}C$, ebulliometry-differential thermal analysis, measured range 105 – $231^{\circ}C$, Kemme & Kreps 1969)
- $\log(P/mmHg) = 6.39379 - 1180.306/(104.321 + t/^{\circ}C)$; temp range 105 – $231^{\circ}C$, or pressure range 5.6 – $757.5\ mmHg$ (Antoine eq., ebulliometry-differential thermal analysis, Kemme & Kreps 1969)
- 1.0* (comparative ebulliometry, measured range 127.261 – $255.2^{\circ}C$, Ambrose & Sprake 1970)
- $\log(P/Pa) = 5.94387 - 1434.755/(T/K - 139.888)$; restricted temp range 127.261 – $194.484^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- $\log(P/Pa) = 5.86571 - 1373.916/(T/K - 147.202)$; temp range 127.16 – $255.2^{\circ}C$ (Antoine eq., comparative ebulliometry, Ambrose & Sprake 1970)
- 124* ($76.23^{\circ}C$, comparative ebulliometry, measured range 349.38 – $406.19\ K$, data fitted to Chebyshev polynomial, Ambrose et al. 1974)
- $\log(P/mmHg) = [-0.2185 \times 13849.2/(T/K)] + 9.115470$; temp range 59.5 – $213.5^{\circ}C$ (Antoine eq., Weast 1972–73)
- 0.5866 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel et al. 1973)
- 1.10 ($20^{\circ}C$, evaporation rate-gravimetric method, Gückel 1982)

$\log(P/\text{kPa}) = 5.76028 - 1315.079/(119.128 + t/^{\circ}\text{C})$, temp range 105–231°C (Antoine eq. derived from exptl. data of Kemme & Kreps 1969, Boublik et al. 1984)

$\log(P/\text{kPa}) = 5.84611 - 1365.892/(124.619 + t/^{\circ}\text{C})$, temp range 127.2–255.2°C (Antoine eq. derived from data of Ambrose & Sprake 1970, Boublik et al. 1984)

$\log(P_{\text{S}}/\text{kPa}) = 17.615 - 6028/(T/\text{K})$; temp range 264–279 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_{\text{L}}/\text{kPa}) = 6.57397 - 1761.308/(-113.992 + T/\text{K})$; temp range 349–410 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_{\text{L}}/\text{kPa}) = 5.8587 - 1374.347/(-147.547 + T/\text{K})$; temp range 405–528 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 111.7949 - 8.3502 \times 10^3/(T/\text{K}) - 34.786 \cdot \log(T/\text{K}) + 3.3682 \times 10^{-10} \cdot (T/\text{K}) + 7.2697 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 268–673 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

2.689 (computer value, Yaws et al. 1991)

3.222 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.98 (HPLC-RT correlation, D'Amboise & Hani 1982)

4.57 (shake flask, Log P Database, Hansch & Leo 1987)

4.57 (recommended, Sangster 1993)

4.57 (shake flask, recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constant, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 11.1.1.14.1

Reported aqueous solubilities of 1-decanol at various temperatures

Barton 1984		Stephenson & Stuart 1986	
IUPAC recommended		shake flask-GC/TC	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
15	32	29.6	210
20	36	40.3	260
25	37	50.0	260
102	10000#	60.3	280
120	8000#	70.2	220
	# tentative	80.2	240
		90.4	230
		mp/ $^{\circ}\text{C}$	5

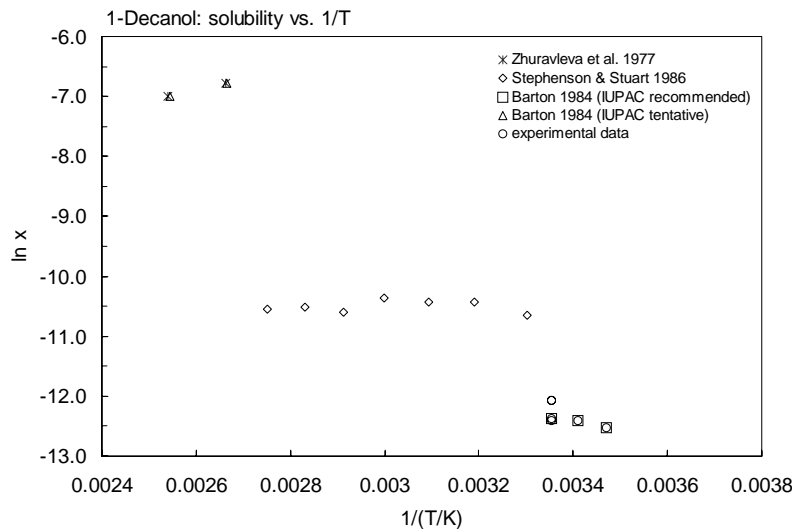


FIGURE 11.1.14.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 1-decanol.

TABLE 11.1.14.2
Reported vapor pressures of 1-decanol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Kemme & Kreps 1969		Ambrose & Sprake 1970		Ambrose & Sprake 1974	
summary of literature data		differential thermal analysis		comparative ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
69.5	133.3	105.0	747	127.261	2656	349.38	124
97.3	666.6	114.5	1360	129.526	2968	358.67	235
111.3	1333	121.7	2000	133.573	3600	364.21	339
125.8	2666	127.3	2680	138.245	4468	364.26	352
142.1	5333	135.6	3986	141.817	5242	371.15	528
152.9	7999	142.2	5346	147.863	6250	371.30	534
165.8	13332	149.9	7466	149.414	7266	375.86	701
186.2	26664	159.2	10812	154.602	8995	379.24	854
208.6	53329	169.9	16172	159.206	10799	380.38	917
231.0	101325	183.9	25398	163.693	12835	383.04	1061
mp/°C	7.0	197.4	40397	168.653	15439	385.72	1236
		215.3	67301	174.653	19146	388.16	1408
		231.0	101005	177.568	21193	392.43	1769
				182.748	25250	395.02	2025
		Antoine eq		189.377	31359	397.42	2283
		eq. 2	P/mmHg	194.484	36807	401.34	2774
		A	6.39397	201.039	44875	403.08	3017

(Continued)

TABLE 11.1.1.14.2 (Continued)

Stull 1947		Kemme & Kreps 1969		Ambrose & Sprake 1970		Ambrose & Sprake 1974	
summary of literature data		differential thermal analysis		comparative ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		B	1180.306	207.352	55899	404.70	3263
		C	104.321	213.119	63364	406.19	3504
				218.923	74244		
				225.489	87994		
				230.471	99886		
				237.598	118863		

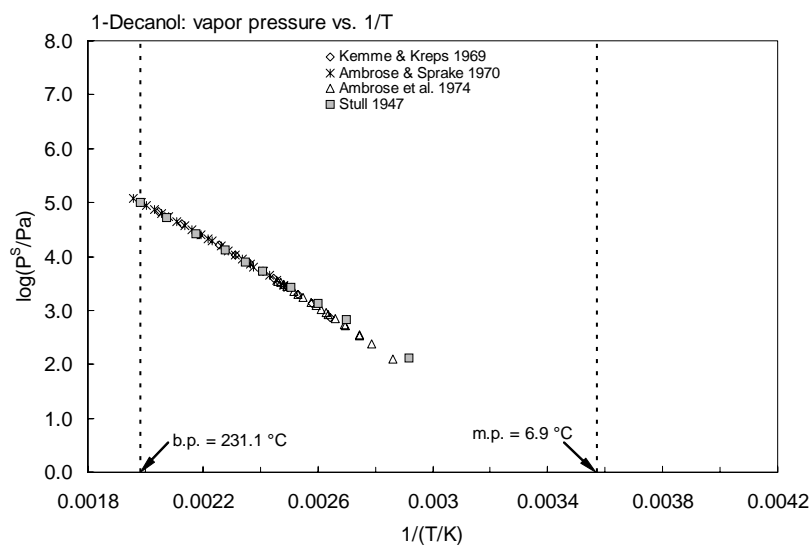
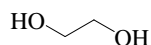


FIGURE 11.1.1.14.2 Logarithm of vapor pressure versus reciprocal temperature for 1-decanol.

11.1.1.15 Ethylene glycol



Common Name: Ethylene glycol

Synonym: 1,2-ethanediol, 1,2-dihydroxyethane, MEG

Chemical Name: 1,2-ethanediol, ethylene glycol

CAS Registry No: 107-21-1

Molecular Formula: $C_2H_6O_2$, $HOCH_2CH_2OH$

Molecular Weight: 62.068

Melting Point ($^{\circ}C$):

−12.69 (Lide 2003)

Boiling Point ($^{\circ}C$):

197.3 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1088 (Weast 1982–83)

Molar Volume (cm^3/mol):

55.8 (Rohrschneider 1973)

66.6 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

14.22 (Dean 1985)

14.24 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.958 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985; Howard 1990; Yaws et al. 1990)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

22.39 (extrapolated-Antoine eq., differential manometer, Gallagher & Hibbert 1937)

$\log(P/mmHg) = 9.2087 - 2976.6/(T/K)$; temp range 40 – $120^{\circ}C$ (Antoine eq. from differential Hg manometry measurements, Gallagher & Hibbert 1937)

133.3* ($53.0^{\circ}C$, summary of literature data, temp range 53.0 – $197.3^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 14032.4/(T/K)] + 9.394685$; temp range: 53 – $197.3^{\circ}C$ (Antoine eq., Weast 1972–73)

11.70* (ebulliometry, extrapolated-Antoine eq., measured range 270 – $310\ K$, Ambrose & Hall 1981)

$\log(P/kPa) = 11.1828 - 2611.2/[(T/K) - 40.0]$; temp range 270 – $310\ K$ (ebulliometry, Antoine eq., Ambrose & Hall 1981)

$\log(P/kPa) = 6.83995 - 1818.591/[(T/K) - 94.499]$; temp range 374.01 – $495.4\ K$ (Antoine eq., ebulliometry, Ambrose & Hall 1981)

7.40* ($20^{\circ}C$, average, gas saturation-GC/FID, Hales et al. 1981)

$\log(P/mmHg) = 23.7259 - 4648.55/(T/K) - 503391/(T/K)^{-2}$; temp range 283 – $373\ K$ (empirical vapor pressure eq., gas saturation, Hales et al. 1981)

14.90 ($20^{\circ}C$, evaporation method, Gückel et al. 1982)

6.67, 26.66 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

0.73, 9.30 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.69339 - 1093.154/(98.821 + t/^{\circ}C)$; temp range 122.5 – $186.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 7.13856 - 2035.185/(1936.936 + t/^{\circ}C)$; temp range 50 – $200^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

11.86 (extrapolated-Antoine eq., Dean 1985)

11.7 (Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.83995 - 1818.591/(178.651 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log (P/\text{kPa}) = 8.3726 - 2994.4/(T/\text{K})$, temp range 130–190°C, (Antoine eq., Riddick et al. 1986)
 $\log (P/\text{mmHg}) = 8.0908 - 2088.9/(203.5 + t/^{\circ}\text{C})$; temp range 50–200°C (Antoine eq., Dean 1985, 1992)
 10.1 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.98465 - 1928.08/(-83.45 + T/\text{K})$; temp range 323–473 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.86912 - 1817.439/(-95.859 + T/\text{K})$, temp range 363–418 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 12.26 (Howard et al. 1986; quoted, Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 82.4062 - 6.3472 \times 10^3/(T/\text{K}) - 25.433 \cdot \log(T/\text{K}) - 2.3732 \times 10^{-9} \cdot (T/\text{K}) + 8.7467 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 160–645 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.006 (calculated- C_W/C_A , Hine & Mookerjee 1975)
 5.81×10^{-6} , 2.37×10^{-5} (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

-1.93 (shake flask, Hansch & Leo 1979)
 -1.34 (shake flask-RC, Cornford 1982)
 -1.36 (shake flask, Log P Database, Hansch & Leo 1987)
 -1.36 (recommended, Sangster 1993)
 -1.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

1.00 (golden ide, after 3 d, Freitag et al. 1985)
 2.28 (algae, after 1 d, Freitag et al. 1985)
 2.30 (activated sludge, after 5 d, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization: evaporation rate $k = 2.915 \times 10^{-6} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined by gravimetric method with an air flow rate $k = (50 \pm 1) \text{ L h}^{-1}$ at $20 \pm 0.1^{\circ}\text{C}$ (Gückel et al. 1973);
 evaporation rate $k = 2.97 \times 10^{-8} \text{ mol cm}^{-2} \text{ h}^{-1}$ was determined at 20°C (Gückel et al. 1982).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 267 \text{ d}$ –64.6 yr in water, based on measured rate constant for the reaction with OH radical (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)
 photooxidation $t_{1/2} = 0.24$ –2.4 h in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)
 $k_{OH} = (7.7 \pm 1.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 295 K in air (Wiedermann & Zetzsch 1982; quoted, Atkinson 1985)
 photooxidation $t_{1/2} = 8.3$ –83 h in air, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991)

Hydrolysis:

Biodegradation:

$k = 41.7 \text{ mg COD g}^{-1} \text{ h}^{-1}$, average rate based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);
 $k = 0.026$ –0.035 h^{-1} in 30 mg/L activated sludge after a time lag of 10–15 h (Urano & Kato 1986b)
 $t_{1/2}(\text{aq. aerobic}) = 48$ –288 h, based on grab sample from river die-away studies (Evans & David 1974; selected, Howard et al. 1991);

$t_{1/2}$ (aq. anaerobic) = 192–1152 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2}$ = 0.24–2.4 h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2}$ = 8.3–83 h, based on measured rate constant for the reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: photooxidation $t_{1/2}$ = 267 d–64.6 yr, based on measured rate constant for the reaction with hydroxyl radicals in water (Anbar & Neta 1967; Dorfman & Adams 1973; quoted, Howard et al. 1991); $t_{1/2}$ = 48–288 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2}$ = 96–576 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ = 48–288 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota

TABLE 11.1.1.15.1

Reported vapor pressures of ethylene glycol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
$\log P = A - B/(T/K) - C/(T/K)^2$	(5)	$\ln P = A - B/(T/K) - C/(T/K)^2$	(5a)

1.

Stull 1947		Ambrose & Hall 1981		Hales et al. 1981			
summary of literature data		comparative ebulliometry		transpiration-GC analysis			
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
				“continuous” measurements		“collection” measurements	
53.0	133.3	100.86	2208	10.0	2.698	9.0	2.711
79.7	666.6	103.869	2584	9.68	2.834	9.8	2.706
92.1	1333	107.59	3121	8.97	2.656	9.79	2.938
105.8	2666	111.997	3885	10.01	7.285	10.02	2.873
120.2	5333	115.971	4705	19.91	7.565	9.73	2.825
129.5	7999	120.647	5857	20.05	7.174	9.94	2.805
141.8	13332	124.645	7032	39.85	14.94	10.09	2.795
158.5	26664	129.735	8800	39.97	43.54	19.9	7.254
178.5	53329	133.244	10244	39.77	42.48	19.05	7.084
197.3	101325	182.095	62918	59.72	44.12	19.93	7.577
		187.372	74338	59.94	184.9	20.51	7.911
mp/ $^{\circ}\text{C}$	–15.6	192.976	88398	60.04	187.8	19.93	7.495
		197.704	101829	59.72	197.8	20.0	7.210
		203.13	119270	74.55	466.2	20.0	7.710
		207.615	135464	74.57	476.9	39.97	41.84
		212.932	156959	73.74	472.6		
		217.989	179863	100.17	2166.0		
		222.287	201399	100.15	2098.0	overall best fit equation	
		25.0	11.70			eq. 5a	
						P/Pa	

(Continued)

TABLE 11.1.1.15.1 (Continued)

Stull 1947		Ambrose & Hall 1981		Hales et al. 1981			
summary of literature data		comparative ebulliometry		transpiration-GC analysis			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		(extrapolated value)				A	23.7259
						B	4648.55
						C	503391
		bp/°C	297.54				
		eq. 3	P/kPa				
		A	6.83995				
		B	1818.591				
		C	-94.499				

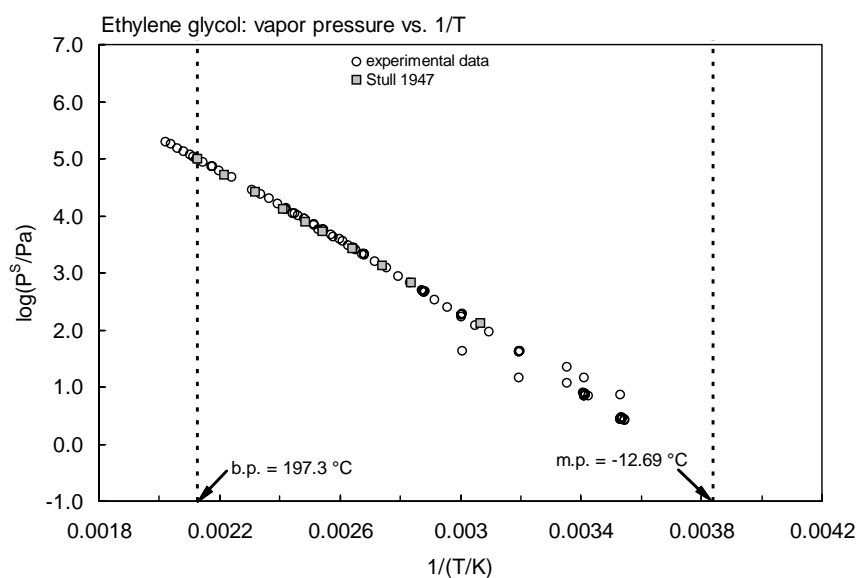
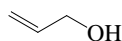


FIGURE 11.1.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for ethylene glycol.

11.1.1.16 Allyl alcohol



Common Name: Allyl alcohol

Synonym: propenylalcohol, 2-propen-1-ol, 1-propene-3-ol, vinylcarbinol

Chemical Name: allyl alcohol, 1-propene-3-ol, 2-propen-1-ol

CAS Registry No: 107-18-6

Molecular Formula: C_3H_6O , $CH_2=CHCH_2OH$

Molecular Weight: 58.079

Melting Point ($^{\circ}C$):

−129 (Stull 1947; Weast 1982–83; Verschueren 1983; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

97.1 (Weast 1982–83; Dean 1985; Riddick et al. 1986)

97 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.854 (Weast 1982–83; Dean 1985)

0.85511 ($15^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

64.8 (Kamlet et al. 1986; Leahy 1986)

74.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

15.5 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2666* ($21.7^{\circ}C$, temp range -20 to $96.6^{\circ}C$, Stull 1947)

3140 (Hoy 1970)

$\log(P/mmHg) = [-0.2185 \times 10577.7/(T/K)] + 9.143231$; temp range -20 to $96.6^{\circ}C$ (Antoine eq., Weast 1972–73)

2666, 4266 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

3750 (Riddick et al. 1986)

$\log(P/kPa) = 31.75070 - 3451.8/(T/K) - 7.94975 \log(T/K)$; temp not specified (Riddick et al. 1986)

3298 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.40725 - 1790.13/(-38.295 + T/K)$; temp range 253 – $370\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 21.3978 - 2.9525 \times 10^3/(T/K) - 3.8137 \cdot \log(T/K) - 2.7145 \times 10^{-3} \cdot (T/K) + 1.8811 \times 10^{-6} \cdot (T/K)^2$; temp range 144 – $545\ K$ (vapor pressure eq., Yaws 1994)

6954* ($38.28^{\circ}C$, ebulliometry, measured range 311.42 – $355.70\ K$, Lubomska & Malanowski 2004)

$\log(P/kPa) = 6.936209 - 1513.129/[(T/K) - 63.131]$; temp range 311.42 – $355.70\ K$ (Antoine eq., ebulliometric method, Lubomska & Malanowski 2004)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.506 (calculated- C_W/C_A , Hine & Mookerjee 1975)

0.510 (calculated-bond contribution, Hine & Mookerjee 1975)

0.564 (computed, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.17 (shake flask, Hansch & Leo 1979)
- 0.17 (recommended, Sangster 1989)
- 0.17 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 334 \text{ d}$ – 37 yr , based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991)

photooxidation $t_{1/2} = 2.2$ – 22 h , based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991)

$k_{OH} = 25.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 440 K (Atkinson 1989)

Biodegradation: $t_{1/2}(\text{aq. aerobic}) = 24$ – 168 h , based on estimated unacclimated aqueous aerobic biodegradation screening test data (Sasaki 1978; quoted, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 96$ – 672 h , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.2$ – 22 h , based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 334 \text{ d}$ – 37 yr , based on measured rate constant for the reaction with hydroxyl radical in water (Anbar & Neta 1967; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ – 336 h , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Sediment:

Soil: $t_{1/2} = 24$ – 168 h , based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 11.1.1.16.1

Reported vapor pressures of allyl alcohol at various temperatures

Stull 1947		Lubomska & Malanowski 2004	
summary of literature data		ebulliometry	
$t/^\circ\text{C}$	P/Pa	T/K	P/Pa
–20.0	133.3	311.42	6954
0.20	666.6	315.81	8869
10.5	1333	319.97	11079
21.7	2666	326.70	15672
33.4	5333	331.84	20194
40.3	7999	334.20	22603
50.0	13332	337.96	26943
64.5	26664	341.54	31723

TABLE 11.1.1.16.1 (Continued)

Stull 1947		Lubomska & Malanowski 2004	
summary of literature data		ebulliometry	
t/°C	P/Pa	T/K	P/Pa
80.2	53329	344.27	35822
96.6	101325	346.97	40304
		351.37	48613
mp/°C	−129	353.15	52334
		353.59	53299
		355.70	58108

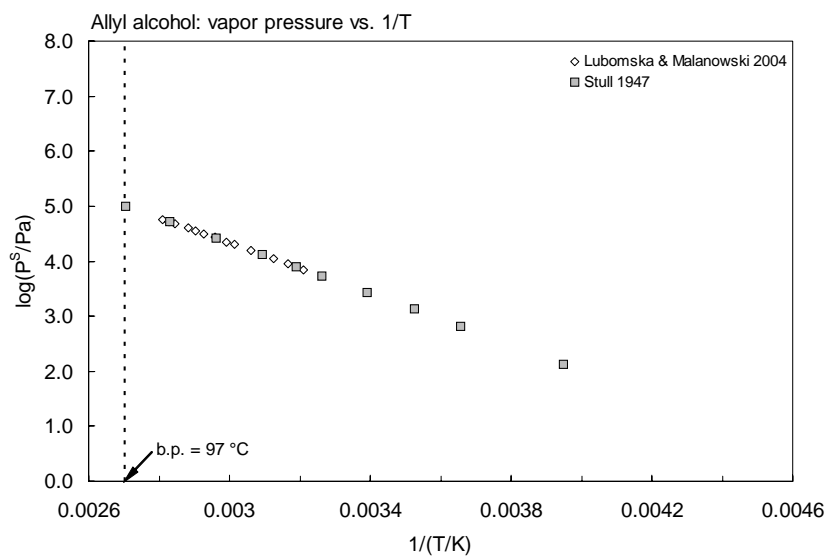
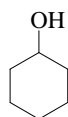


FIGURE 11.1.1.16.1 Logarithm of vapor pressure versus reciprocal temperature for allyl alcohol.

11.1.1.17 Cyclohexanol



Common Name: Cyclohexanol

Synonym: adronol, anol, cyclohexylalcohol, hexahydrophenol, hexalin, hydralin, hydrophenol

Chemical Name: cyclohexanol

CAS Registry No: 108-93-0

Molecular Formula: $C_6H_{11}OH$

Molecular Weight: 100.158

Melting Point ($^{\circ}C$):

25.93 (Lide 2003)

Boiling Point ($^{\circ}C$):

160.84 (Lide 2003)

Density (g/cm^3):

0.9624 (Lide 2003)

Molar Volume (cm^3/mol):

104.0 (calculated-density, Lande & Banerjee 1981)

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

1.70 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

37000* (shake flask-synthetic method, temp range 7.2 – $184.72^{\circ}C$, Sidgwick & Sutton 1930)

39200 (shake flask-interferometry, Hansen et al. 1949)

32920 (residue volume, Booth & Everson 1942)

40000* ($20^{\circ}C$, synthetic method, measured range 0 – $184^{\circ}C$, Zil'berman 1951)

48960 (shake flask-interferometry, Donahue & Bartell 1952)

36000 ($26.7^{\circ}C$, shake flask-turbidity, Skrzec & Murphy 1954)

38000* (recommended "best" value, IUPAC Solubility Data Series, temp range 0 – $180^{\circ}C$, Baron 1984)

37500 (selected, Riddick et al. 1986)

44400* ($19.7^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.3^{\circ}C$, Stephenson & Stuart 1986)

38200 (selected, Yaws et al. 1990)

37500 (dialysis tubing equilibration-GC. Etzweiler et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

467* ($34.0^{\circ}C$, Ramsay-Young method, measured range 34.0 – $149.0^{\circ}C$, Gardner & Brewer 1937)

133.1*, 194 ($21^{\circ}C$, interpolated-regression of tabulated data, temp range 21 – $161^{\circ}C$, Stull 1947)

7177* ($93.73^{\circ}C$, temp range 93.73 – $160.70^{\circ}C$, Novak et al. 1960; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 11935.8/(T/K)] + 8.909086$; temp range 21 – $161^{\circ}C$ (Antoine eq., Weast 1972–73)

174.8 (calculated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 434.658/(T/K)] \times 10^{\{0.951396 - 8.46102 \times 10^{-4} \cdot (T/K) + 8.87926 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 294.15 – $434.15\ K$ (Cox eq., Chao et al. 1983)

37.53 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.2553 - 912.87/(109.13 + t/^{\circ}C)$; temp range 94 – $161^{\circ}C$ (Antoine eq., Dean 1985, 1992)

1300 ($56^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 5.92859 - 1199.10/(t/^{\circ}C + 145.0)$; temp range 107 – $160^{\circ}C$ (Riddick et al. 1986)

97.36 (interpolated, solid, Antoine eq.-I, Stephenson & Malanowski 1987)

80.0, 84.85 (extrapolated, liquid, Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 9.631 - 3173.1/(T/\text{K})$; temp range 272–298 K (Antoine eq.-I, for solid, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.1634 - 1318.5/(-116.55 + T/\text{K})$; temp range 318–434 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.27792 - 1381.8/(-110.132 + T/\text{K})$; temp range 300–434 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

106.6 (Daubert & Danner 1989)

14.66, 196.0 (quoted, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 49.9123 - 4.8446 \times 10^3/(T/\text{K}) - 13.711 \cdot \log(T/\text{K}) + 3.5451 \times 10^{-9} \cdot (T/\text{K}) + 1.5932 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 297–625 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

0.581 (calculated- C_w/C_A , Hine & Mookerjee 1975)

2.48, 2.37 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

0.281 (calculated-P/C, Howard 1993)

0.278 (correlated-molecular structure, Russell et al. 1992)

0.446 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.23 (shake flask-AS, Hansch & Anderson 1967, Hansch et al. 1968; Leo et al. 1971; Hansch & Leo 1979)

1.36 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)

1.23 (recommended, Sangster 1989, 1993)

1.23 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

5.18 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

0.708 (estimated- K_{ow} , Lyman et al. 1990)

0.176 (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

2.045 (soil, estimated- K_{ow} , Lyman et al. 1990; quoted, Howard 1993)

1.114 (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 145$ d estimated from a model environmental pond with the consideration of the effect of adsorption (USEPA 1987; quoted, Howard 1993);

based on the Henry's law constant, $t_{1/2} \sim 13.3$ d from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s at 25°C (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 17.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with OH radical concentration of 5×10^5 per cm^3 in air at 25°C corresponds to an atmosphere $t_{1/2} = 22$ h (Atkinson 1987; quoted, Howard 1993)

Hydrolysis:

Biodegradation: average rate of biodegradation $k = 28.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 22$ h, based on estimated reaction rate constant of 17.4×10^{-12} cm³ molecule⁻¹ s⁻¹ for the vapor phase reaction with 5×10^5 hydroxyl radical per cm³ in air at 25°C (Howard 1993).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 11.1.1.17.1

Reported aqueous solubilities of cyclohexanol at various temperatures

Sidgwick & Sutton 1930		Zil'berman 1951		Barton 1984		Stephenson & Stuart 1986	
synthetic method		synthetic method		IUPAC recommended		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
7.2	50000	0	53400	0	53000	0	67700
9.4	47800	10	45700	10	46200	9.5	54000
9.7	45800	20	40000	20	39700	19.7	44400
11.2	44100	30	36000	25	38000	30.6	37400
12.0	45500	40	33300	30	35500	40.0	36300
14.2	42300	50	31400	40	33000	50.0	34900
15.2	42900	54	31000	50	31000	60.3	33700
16.3	40900	62	31000	60	31000	70.1	34400
20.6	39500	70	31900	70	32000	80.2	36000
20.8	38200	80	34100	80	34000	90.3	37500
24.6	37500	90	36500	90	37000		
27.55	35200	100	39300	100	39000		
28.7	35700	110	42800	110	43000		
31.85	33700	120	47000	120	49000		
33.6	34100	130	53000	130	56000		
40.4	32600	140	61000	140	64000		
40.45	31800	150	72000	150	77000		
45.8	31900	160	88000	160	93000		
121.95	51400	170	115000	170	120000		
156.9	92200	180	178000	180	190000		
174.3	150000	184	339000				
179.4	192000						
184.72	324000						

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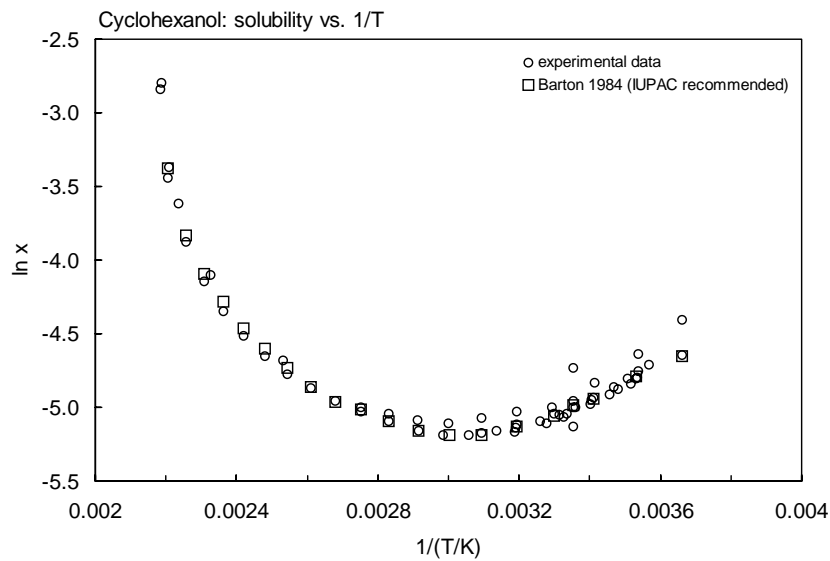


FIGURE 11.1.1.17.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for cyclohexanol.

TABLE 11.1.1.17.2
Reported vapor pressures of cyclohexanol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$

(1)

$\log P = A - B/(C + t/^{\circ}\text{C})$

(2)

$\log P = A - B/(C + T/K)$

(3)

$\log P = A - B/(T/K) - C \cdot \log (T/K)$

(4)

$\ln P = A - B/(T/K)$

(1a)

$\ln P = A - B/(C + t/^{\circ}\text{C})$

(2a)

Gardner & Brewer 1937		Stull 1947		Novak et al. 1960	
Ramsay-Young method		summary of literature data		in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
34.0	467	21.0	133.3	93.73	7177
37.5	560	44.0	666.6	97.02	9210
46.4	587	56.0	1333	99.71	10426
47.8	693	68.8	2666	102.52	11876
53.6	907	83.0	5333	104.83	13159
59.4	1133	91.8	7999	108.82	15372
73.0	2773	103.7	13332	112.70	18252
80.5	4146	121.7	26664	116.86	21891
97.8	9826	141.4	53329	120.35	25264
119.1	13771	161.0	101325	125.54	30864
136.9	47036			130.95	37543
149.0	71994	mp/°C	23	136.22	45356
				142.41	56448
bp/°C	162.3			148.72	69487
				155.71	86046
				160.70	99192
				in Boublik et al. 1984	
				eq. 2	P/kPa
				A	5.34182
				B	894.818
				C	106.797
				bp/°C	161.425

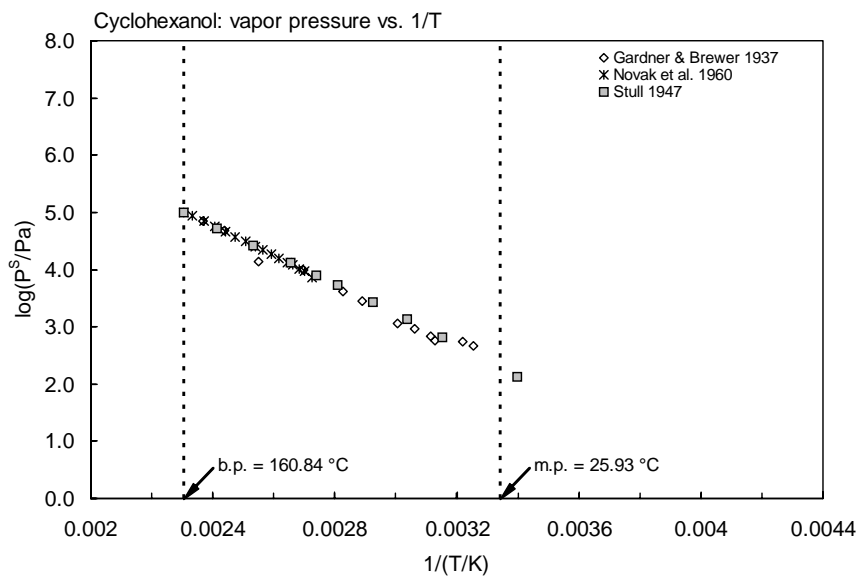
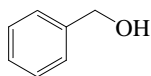


FIGURE 11.1.17.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexanol.

11.1.1.18 Benzyl alcohol



Common Name: Benzyl alcohol

Synonym: benzenemethanol, (hydroxymethyl)benzene, *o*-hydroxy toluene, phenylcarbinol, phenylmethanol

Chemical Name: benzyl alcohol

CAS Registry No: 100-51-6

Molecular Formula: C_7H_8O , $C_6H_5CH_2OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

-15.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

205.31 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.04535, 1.04156 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

1.04127 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

103.5 (calculated-density, Rohrschneider 1973)

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

48.13, 61.42 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.406 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

38020 (Seidell 1941)

34200 (estimated, McGowan 1954)

38000 (20 – $25^{\circ}C$, shake flask-GC, Urano et al. 1982)

35000 ($20^{\circ}C$, Verschueren 1983)

42900 (shake flask-LSC, Banerjee 1985)

43000* ($20.1^{\circ}C$, shake flask-GC/TC, measured range 0 – $50^{\circ}C$, Stephenson & Stuart 1986)

46070 (shake flask-GC, Li et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($60.9^{\circ}C$, static method, measured range 60.9 – $152.1^{\circ}C$, Kahlbaum 1898)

26.7* ($38.8^{\circ}C$, ebulliometry, measured range 38.8 – $151.6^{\circ}C$, Gardner & Brewer 1937)

15.40* (extrapolated-regression of tabulated data, temp range 58 – $205.7^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.90550 - 2187.8/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

6287* ($122.52^{\circ}C$, ebulliometry, measured range 122.52 – $205.41^{\circ}C$, Dreisbach & Shrader 1949)

19.59 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.58200 - 1904.3/(200.0 + t/^{\circ}C)$; temp range 112 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

12.0 (Hoy 1970)

$\log(P/mmHg) = [-0.2185 \times 14093.2/(T/K)] + 9.391874$; temp range 58 – $204.7^{\circ}C$ (Antoine eq., Weast 1972–73)

8.35*, 10.06 ($20^{\circ}C$, $25^{\circ}C$, extrapolated-Antoine eq., gas-saturation method, Grayson & Fosbraey 1982)

$\log(P/Pa) = 29.0 - 7958/(T/K)$; temp range 29.5 – $60.1^{\circ}C$ (Antoine eq., gas saturation, Grayson & Fosbraey 1982)

4.750 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/\text{mmHg}) = [1 - 479.624/(T/K)] \times 10^{1.02742 - 6.26739 \times 10^{-4} \cdot (T/K) + 1.28791 \times 10^{-7} \cdot (T/K)^2}$; temp range 340.95–463.65 K (Cox eq., Chao et al. 1983)
 12.07, 9.69 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.34897 - 1650.313/(174.623 + t/^{\circ}\text{C})$; temp range 122.5–205.4°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.39383 - 1655.003/(171.85 + t/^{\circ}\text{C})$; temp range 38.8–151.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 11.72 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.19817 - 1632.593/(172.79 + t/^{\circ}\text{C})$; temp range 122–205°C (Antoine eq., Dean 1985, 1992)
 15.0 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 8.963 - 3214/(T/K)$; temp range not specified (Antoine eq., Riddick et al. 1986)
 15.25 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.7069 - 1904.3/(-73.15 + T/K)$; temp range 385–573 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.963 - 3214/(T/K)$; temp range 293–315 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 7.395 (ebulliometry, fitted to Antoine eq., Ambrose & Ghassee 1990)
 12.0 (calculated-Wagner eq., Ambrose & Ghassee 1990)
 $\log (P/\text{mmHg}) = -36.2189 - 3.3475 \times 10^3/(T/K) + 23.337 \cdot \log(T/K) - 4.46 \times 10^{-2} \cdot (T/K) + 2.1443 \times 10^{-5} \cdot (T/K)^2$; temp range 258–677 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.0231 (quoted estimated value of Hine & Mookerjee 1975, Howard 1993)
 0.0396 (calculated-P/C, Howard 1993)
 < 0.0273 (wetted-wall column-GC, Altschuh et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.10 (shake flask-UV, Fujita et al. 1964; Hansch et al. 1968)
 1.10 ± 0.02 (shake flask-UV, Iwasa et al. 1965)
 1.10 (shake flask-UV, Hansch et al. 1968)
 1.10 (shake flask-RC, Cornford 1982)
 1.00 (shake flask-UV, Mayer et al. 1982)
 1.16 ± 0.02 (exptl.-ALPM, Garst & Wilson 1984)
 1.06 (HPLC-k' correlation, Eadsforth 1986)
 1.58 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 1.05 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
 1.05 (recommended, Sangster 1989, 1993)
 1.22 (centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)
 0.96 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)
 1.10 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.602 (calculated- K_{ow} , Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{oc}$:

1.193 (red-brown Australian soil with 1.09% organic carbon, Briggs 1981; quoted, Howard 1993)
 0.790 (calculated- K_{ow} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 97$ d for a model river of 1 m deep, flowing at 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 7.99 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated from Atmospheric Oxidation Program; $k_{\text{OH}}(\text{exptl}) = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{\text{OH}}(\text{calc}) = 7.98 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, estimated from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)

$k_{\text{OH}}(\text{calc}) = 0.85 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{exptl}) = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: biodegradation rate constant $k = 0.042\text{--}0.062 \text{ h}^{-1}$ in 30 mg L⁻¹ activated sludge after a lag time of 5–15 h (Urano & Kato 1986).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: the estimated $t_{1/2} \sim 2 \text{ d}$ for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere (Atkinson 1985; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 11.1.1.18.1

Reported aqueous solubilities of benzyl alcohol at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC	
t/°C	S/g·m ⁻³
0	48000
9.8	47000
20.1	43000
29.6	43000
40.2	45000
50.0	52000

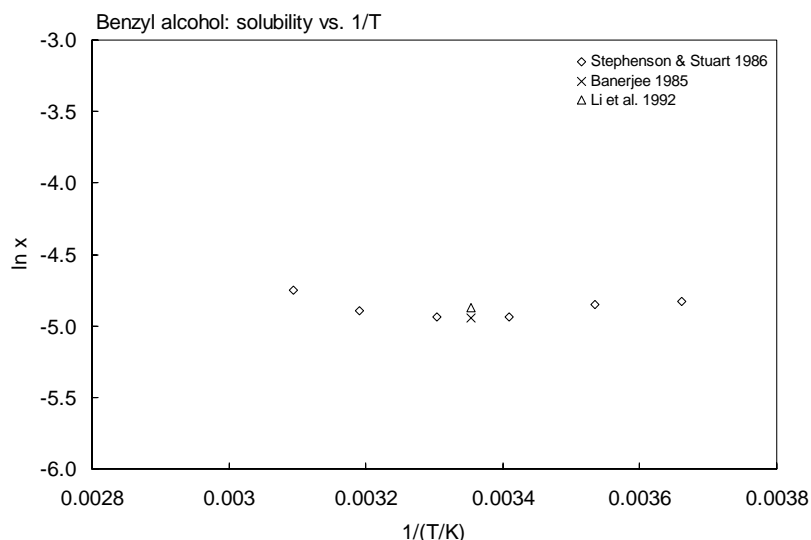


FIGURE 11.1.1.18.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for benzyl alcohol.

TABLE 11.1.1.18.2

Reported vapor pressures of benzyl alcohol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Kahlbaum 1898		Gardner & Brewer 1937		Stull 1947		Grayson & Fosbraey 1982	
static method		ebulliometry		summary of literature data		gas saturation-GC/LC	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
60.9	133.3	38.8	26.7	58.0	133.3	29.5	18.29
67.8	266.6	42.5	80.0	80.8	666.6	30.2	22.77
72.9	400.0	46.8	106.7	92.6	1333	39.8	44.22
77.2	533.3	50.5	120.0	105.8	2666	40.1	46.11
80.8	666.6	85.2	906.6	119.8	5333	49.7	101.41
92.8	1333.2	97.2	1747	129.3	7999	60.1	221.10
99.9	1999.8	113.5	3880	141.7	13332	20	8.35
105.3	2666.4	128.8	7786	160.0	26664		
109.7	3333.06	151.6	18918	183.0	53329	eq. 1a	P/Pa
113.4	3999.7			204.7	101325	A	29.0
116.7	4666.3	bp/°C	206.9			B	7958
119.6	5332.9			mp/°C	−15.3		
122.2	5999.5						
124.4	6666.1						
133.9	9999.2						
141.3	13332						
152.1	19998						
				Dreisbach & Shrader 1949			
				ebulliometry			
				t/°C	P/Pa		
				122.52	6287		
				127.12	7605		
				130.90	8851		
				134.28	10114		
				147.09	16500		
				190.50	67661		
				205.41	101325		

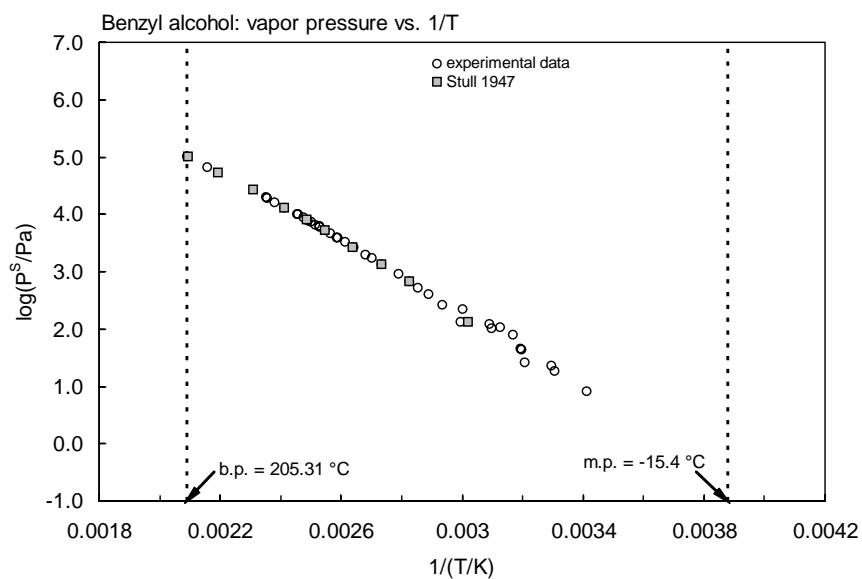


FIGURE 11.1.18.2 Logarithm of vapor pressure versus reciprocal temperature for benzyl alcohol.

11.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 11.2.1
Summary of physical properties of alcohols

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C	Molar volume, V_M cm ³ /mol	
							MW/ ρ at 20°C	Le Bas
Methanol	67-56-1	CH ₃ OH	32.042	-97.53	64.6	1	40.49	37.0
Ethanol	64-17-5	C ₂ H ₅ OH	46.068	-114.14	78.29	1	58.36	59.2
Propanol (<i>n</i> -Propyl alcohol)	71-23-8	C ₃ H ₇ OH	60.095	-124.39	97.2	1	74.79	81.4
Isopropanol (<i>i</i> -Propyl alcohol)	67-63-0	<i>i</i> C ₃ H ₇ OH	60.095	-87.9	82.3	1	76.51	81.4
1-Butanol (<i>n</i> -Butyl alcohol)	71-36-3	C ₄ H ₉ OH	74.121	-88.6	117.73	1	91.56	103.6
Isobutanol (<i>i</i> -Butyl alcohol)	78-83-1	<i>i</i> C ₄ H ₉ OH	74.121	-101.9	107.89	1	92.47	103.6
<i>sec</i> -Butyl alcohol	78-92-2	<i>s</i> C ₄ H ₉ OH	74.121	-88.5	99.51	1	91.90	103.6
<i>tert</i> -Butyl alcohol	75-65-0	<i>t</i> C ₄ H ₉ OH	74.121	25.69	82.4	1	94.88	103.6
1-Pentanol (<i>n</i> -Amyl alcohol)	71-41-0	C ₅ H ₁₁ OH	88.148	-77.6	137.98	1	108.23	125.8
2-Pentanol	6032-29-7	C ₅ H ₁₁ OH	88.148	-73	119.3	1	108.91	125.8
1-Hexanol	111-27-3	C ₆ H ₁₃ OH	102.174	-47.4	157.6	1	124.79	148.0
1-Heptanol	111-70-6	C ₇ H ₁₅ OH	116.201	-33.2	176.45	1	141.38	170.2
1-Octanol (<i>n</i> -Octyl alcohol)	111-87-5	C ₈ H ₁₇ OH	130.228	-14.8	195.16	1	157.85	192.4
1-Nonanol	143-08-8	C ₉ H ₁₉ OH	144.254	-5	213.37	1	174.37	214.6
1-Decanol	112-30-1	C ₁₀ H ₂₁ OH	158.281	6.9	231.1	1	190.77	236.8
Ethylene glycol	107-21-1	(CH ₂ OH) ₂	62.068	-12.69	197.3	1	55.98	66.6
Allyl alcohol	107-18-6	C ₃ H ₅ OH	58.079	-129	97	1	67.92	74.0
Cyclopentanol	96-41-3	C ₅ H ₉ OH	86.132	-17.5	140.42	1	90.78	106.9
Cyclohexanol	108-93-0	C ₆ H ₁₁ OH	100.158	25.93	160.84	1	104.07	125.6
Benzyl alcohol	100-51-6	C ₇ H ₇ OH	108.138	-15.4	205.31	1	103.85	125.6

TABLE 11.2.2
Summary of selected physical-chemical properties of alcohols at 25°C

Compound	Selected properties				Henry's law constant H/(Pa·m³/mol)			
	Solubility		Vapor pressure		log K _{OW} calcd P/C	exptl (a)	exptl (b)	exptl (c)
	S/(g/m³)	C _L /(mol/m³)	P _L /Pa					
Methanol	miscible	miscible	16210	−0.77		0.45		0.45
Ethanol	miscible	miscible	7800	−0.31		0.53		0.527
Propanol	miscible	miscible	2780	0.25				0.751
Isopropanol	miscible	miscible	5700	0.05				0.80
1-Butanol	74000	998.4	900	0.82	0.9014	0.80	0.892	0.80
Isobutanol	81000	1093	1500	0.76	1.3726	0.99		0.99
<i>sec</i> -Butyl alcohol	181000	2442	2300	0.61	0.9419	0.80		0.918
<i>tert</i> -Butyl alcohol	miscible	miscible	5500	0.35		1.46		1.46
1-Pentanol	22000	249.6	300	1.50	1.202	1.314		
2-Pentanol	45000	510.5	777	1.14	1.522			
1-Hexanol	6000	58.72	110	2.03	1.873	1.562	1.735	
1-Heptanol	1740	14.97	24	2.62	1.603	1.909		
1-Octanol	540	4.146	11	3.07	2.653	2.454	2.48	
1-Nonanol	130	0.9012		4.26				
1-Decanol	37	0.2338		4.57				
Ethylene glycol	miscible	miscible	12	−1.36		0.006		
Allyl alcohol	miscible	miscible	3750	0.17				
Cyclopentanol			292					
Cyclohexanol	38000	379.4	85	1.23	0.224			
Benzyl alcohol	80	0.7398	12	1.10	16.22			

(a) Butler et al. 1935

(b) Buttery et al. 1969

(c) Snider & Dawson 1985

TABLE 11.2.3

Suggested half-life classes of alcohols in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Methanol	4	3	3	4
Ethanol	3	3	3	4
Propanol (<i>n</i> -Propyl alcohol)	3	3	3	4
Isopropanol (<i>i</i> -Propyl alcohol)	3	3	3	4
1-Butanol (<i>n</i> -Butyl alcohol)	3	3	3	4
Isobutanol (<i>i</i> -Butyl alcohol)	3	3	3	4
<i>tert</i> -Butyl alcohol	4	4	4	5
1-Pentanol (<i>n</i> -Amyl alcohol)	3	3	3	4
1-Hexanol	3	3	3	4
1-Octanol (<i>n</i> -Octyl alcohol)	3	3	3	4
Ethylene glycol	3	3	3	4
Allyl alcohol	3	3	3	4
Cyclohexanol	3	3	3	4
Benzyl alcohol	3	3	3	4

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

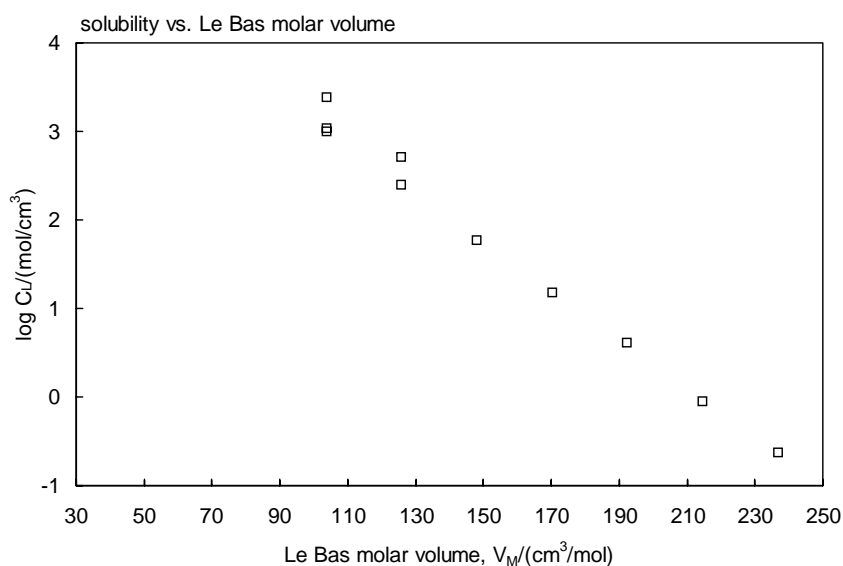


FIGURE 11.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.

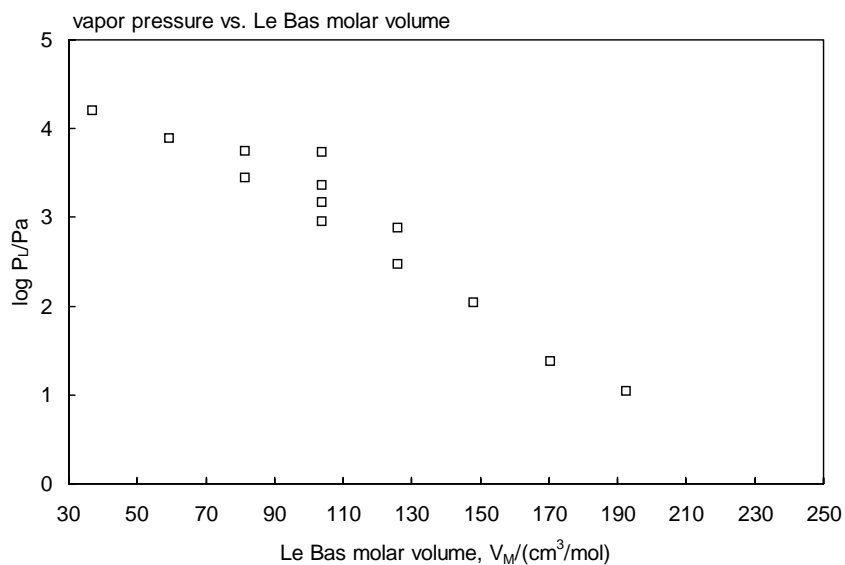


FIGURE 11.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for alcohols.

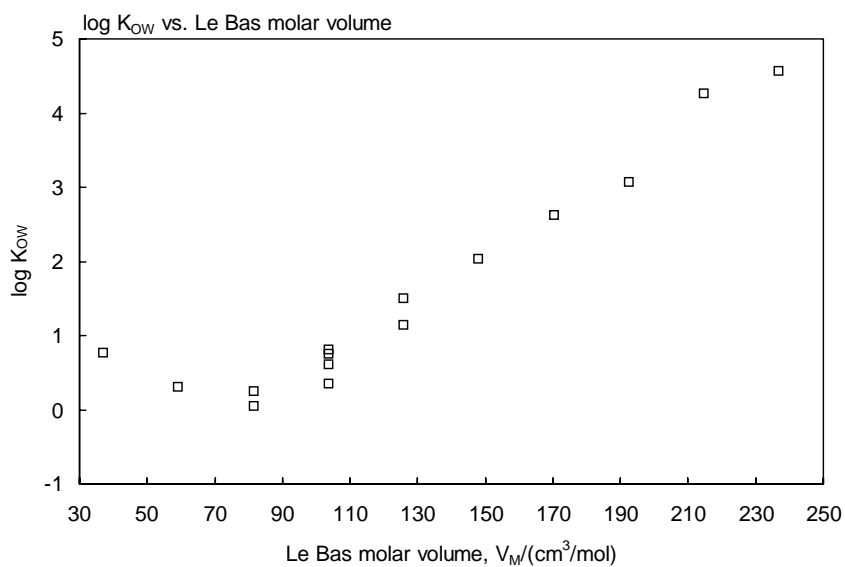


FIGURE 11.2.3 Octanol-water partition coefficient versus Le Bas molar volume for alcohols.

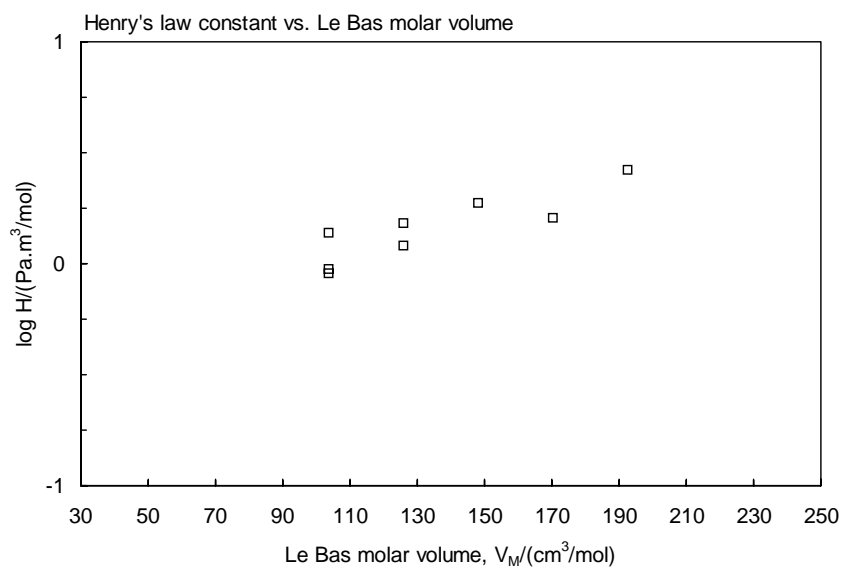


FIGURE 11.2.4 Henry's law constant versus Le Bas molar volume for alcohols.

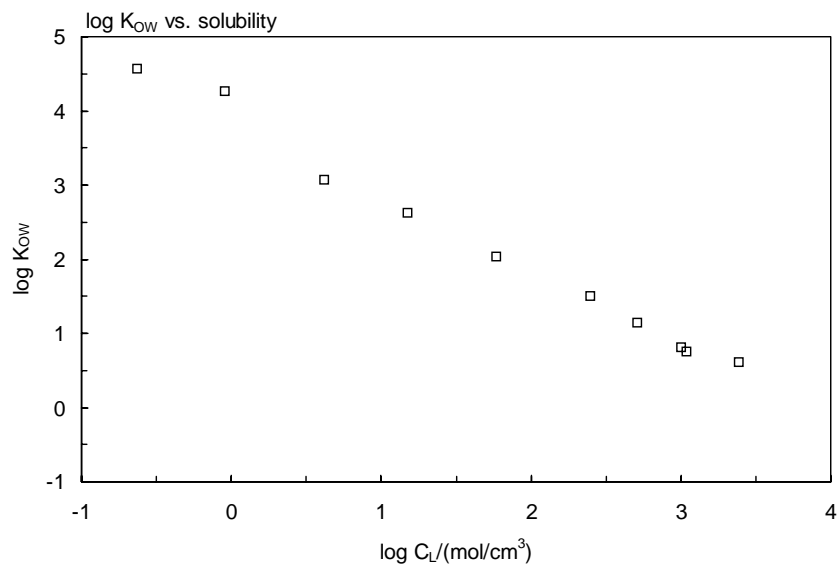


FIGURE 11.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for alcohols.

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12 Aldehydes and Ketones

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12.1 LIST OF CHEMICALS AND DATA COMPILATIONS

12.1.1 ALDEHYDES

12.1.1.1 Methanal (Formaldehyde)



Common Name: Formaldehyde

Synonym: formalin, methanal, oxomethane

Chemical Name: formaldehyde

CAS Registry No: 50-00-0

Molecular Formula: CH₂O, HCHO

Molecular Weight: 30.026

Melting Point (°C):

-92.0 (Weast 1982–83; Dean 1985; Lide 2003)

Boiling Point (°C):

-19.1 (Lide 2003)

Density (g/cm³):

0.815 (-20°C, Weast 1982–83)

0.815 (-20°C, Verschuereen 1983; Dean 1985)

Molar Volume (cm³/mol):

36.8 (-20°C, Stephenson & Malanowski 1987)

29.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K.), F: 1.0Water Solubility (g/m³ or mg/L at 25°C):

1220000 (Dean 1985)

very soluble, up to 55% (Budavari 1989, Howard 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

88566* (-22.29°C, static method-differential manometer, measured range -109.39 to -22.29°C, Spencer & Wild 1935)

101325* (-19.5°C, summary of literature data, temp range -88 to -19.5°C, Stull 1947)

log (P/mmHg) = [-0.2185 × 5917.9/(T/K)] + 7.985746; temp range -88 to -19.5°C (Antoine eq., Weast 1972–73)

1333 (-88°C, Verschuereen 1983)

log (P/kPa) = 6.32524 - 972.5/(244.329 + t/°C), temp range (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 7.1958 - 970.65/(244.1 + t/°C); temp range -109 to -22°C (Antoine eq., Dean 1985, 1992)

log (P_L/kPa) = 6.5475 - 1062.4/(-19.92 + T/K), temp range 184–251 K (Antoine eq.-I, Stephenson & Malanowski 1987)

log (P_L/kPa) = 6.4306 - 1013.206/(-24.883 + T/K); temp range 163–251 K (Antoine eq.-II, Stephenson & Malanowski 1987)

517690 (1 atm, Howard 1989)

log (P/mmHg) = 41.9603 - 2.1355 × 10³/(T/K) - 13.765·log (T/K) + 9.568 × 10⁻³·(T/K) - 5.1101 × 10⁻¹²·(T/K)²; temp range 181–408 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0331 (20°C, porous membrane gas-liquid equilibration system, Dong & Dasgupta 1986)

0.0169 (review, Gaffney et al. 1987)

0.0341* (gas stripping-headspace GC, measured range 15–45°C, Betterton & Hoffmann 1988)

0.0298* (gas-stripping-HPLC-UV, freshwater, measured range 10–45°C, Zhou & Mopper 1990)

$\ln [K_H'/(M/atm)] = -6.0 + 2844/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

$\ln [K_H'/(M/atm)] = -6.7 + 3069/(T/K)$, temp range 25–45°C (gas stripping-HPLC measurements, seawater (salinity $35 \pm 1\%$), Zhou & Mopper 1990)

0.021 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.621 - 2840/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.35 (shake flask, Johnson & Piret 1948)

–1.54 (Kenaga & Goring 1980)

0.00 (Verschuere 1983)

0.35 (recommended, Sangster 1989)

0.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

no bioconcentration. in fish and shrimp observed (Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: sunlight photolysis $t_{1/2} = 1.25$ – 6.0 h, based on measured gas-phase photolysis by simulated sunlight (Calvert et al. 1972; Su et al. 1979; quoted, Howard et al. 1991);

rate constant $k = 8.0 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986);

calculated lifetime of 4 h (Atkinson 2000).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius equation see reference:

$k_{OH} = 1.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

aqueous photooxidation $t_{1/2} = 4813$ – 190000 h, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; quoted, Howard et al. 1991)

$k_{OH} = 1.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (long-path Fourier transform IR, Niki et al. 1978)

$k_{NO_3} = 3.2 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 1 K (review, Atkinson & Lloyd 1984)

$k = (0.1 \pm 0.03) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{HO_2} = 4.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with HO_2 radical at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

$k_{OH} = 1.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

$k_{OH}(\text{calc}) = 7.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 9.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

atmospheric photooxidation half-life of 7.13–71.3 h, based on measured rate constant for the vapor-phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991)

$k_{OH}^* = 9.77 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{NO_3} = 5.8 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{OH}(\text{calc}) = 17.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: degradation complete in 20 h under aerobic conditions and 48 h under anaerobic conditions in a die-away test using water from a stagnant lake (Howard 1989)

aqueous aerobic half-life of 24–168 h, based on unacclimated aqueous aerobic biodegradation screening test data; aqueous anaerobic half-life of 96–672 h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: half-life is a few hours in the sunlit troposphere; $t_{1/2} = 19$ and 50 h by dry deposition and wet removal, respectively; $t_{1/2} = 12$ d when reacts with NO_3 radical by H-atom abstraction. (Howard 1989)

photooxidation $t_{1/2} = 7.13\text{--}71.3$ h, based on measured rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

$t_{1/2} = 1.26\text{--}6.0$ h, based on photolysis half-life in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994);

calculated lifetimes of 1.2 d, 80 d and > 4.5 yr for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.1.1.1

Reported vapor pressures of methanal (formaldehyde) at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Spencer & Wild 1935		Stull 1947	
differential manometer		summary of literature data	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-109.39	127	-88.0	1333
-104.39	237	-79.6	2666
-98.29	480	-70.6	5333
-95.19	647	-65.0	7999
-89.09	1157	-57.3	13332
-85.59	1633	-46.0	26664
-78.89	2802	-33.0	53329
-78.29	2946	-19.5	101325
-71.29	4720		
-68.55	6190	mp/ $^{\circ}\text{C}$	-92
-65.29	7859		
-64.59	8219		
-63.69	8693		
-55.79	14799		
-53.99	16625		
-49.29	21745		
-40.59	35544		
-39.09	38743		
-34.29	49182		
-28.39	66208		
-22.29	88566		

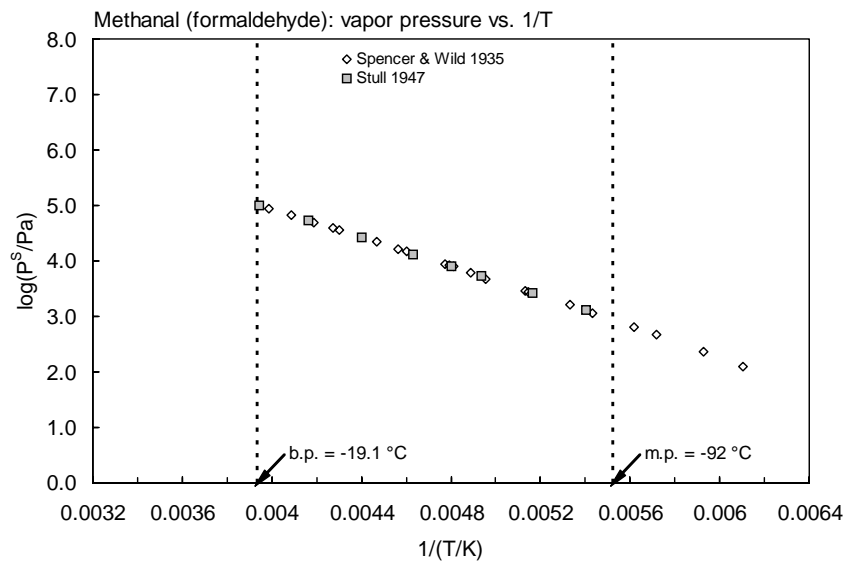


FIGURE 12.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methanal.

TABLE 12.1.1.1.2
Reported Henry's law constants of methanal (formaldehyde) at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$

(1)

$$\ln (1/K_{AW}) = A - B/(T/K)$$

(2)

$$\ln (k_H/\text{atm}) = A - B/(T/K)$$

(3)

$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$

(4)

$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

(5)

$$\log K_{AW} = A - B/(T/K)$$

(1a)

$$\log (1/K_{AW}) = A - B/(T/K)$$

(2a)

$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

(4a)

Betterton & Hoffmann 1988		Zhou & Mopper 1990			
gas stripping-fluorescence		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
		fresh water		sea water	
15	0.01386	10	0.01023	10	0.0074
15	0.01031*	17	-	17	0.0128
25	0.0341	25	0.0298	25	0.0284
35	0.0675	30	0.0507	30	0.0405
45	0.1506	35	0.0675	35	0.0533
		40	0.0921	40	-
		45	0.125	45	0.115
$\Delta H/(\text{kJ mol}^{-1}) = -59.8$					
* in 0.5 M HSO ₄ solution		eq. 1a	K _H '/(M/atm)	eq. 1a	K _H '/(M/atm)
		A	-6.00	A	-6.70
		B	-2844	B	-3069

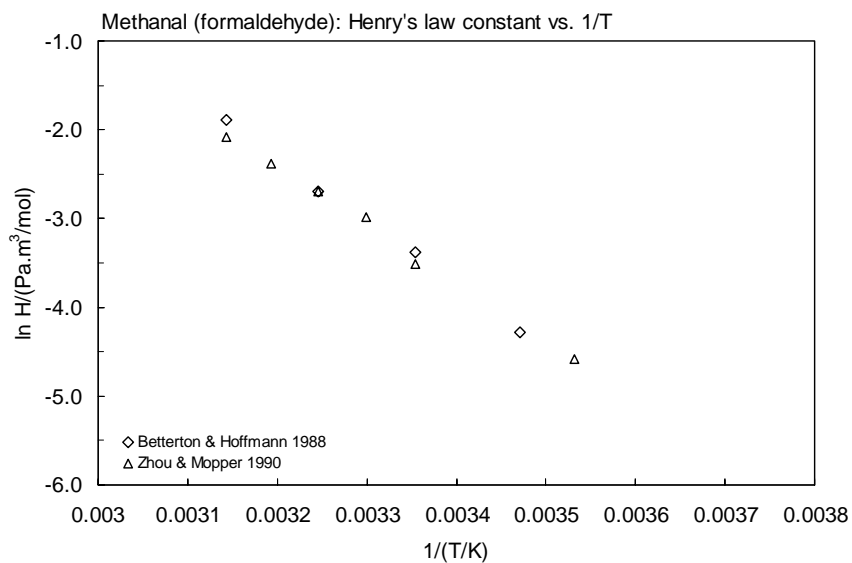


FIGURE 12.1.1.1.2 Logarithm of Henry's law constant versus reciprocal temperature for methanal.

12.1.1.2 Ethanal (Acetaldehyde)



Common Name: Acetaldehyde

Synonym: acetic aldehyde, aldehyde, ethanal, ethylaldehyde

Chemical Name: acetaldehyde, ethanal

CAS Registry No: 75-07-0

Molecular Formula: C_2H_4O , CH_3CHO

Molecular Weight: 44.052

Melting Point ($^{\circ}C$):

−123.37 (Lide 2003)

Boiling Point ($^{\circ}C$):

20.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7834 ($18^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

56.23 ($18^{\circ}C$, calculated-density)

51.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

−10.2 (pK_b , Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

3.243 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Palit 1947; Riddick et al. 1986)

miscible (Verschuereen 1983; Dean 1985)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

101300* ($20.2^{\circ}C$, summary of literature data, temp range -81.5 to $5.9^{\circ}C$, Stull 1947)

102125* ($20.7^{\circ}C$, measured range -0.20 to $34.4^{\circ}C$, Coles & Popper 1950)

120060 (Hoy 1970)

$\log (P/mmHg) = [-0.2185 \times 7267.8/(T/K)] + 8.327803$; temp range -81.5 to $20.2^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [-0.2185 \times 6622.1/(T/K)] + 7.82060$; temp range -24.3 to $27.5^{\circ}C$ (Antoine eq., Weast 1972–73)

98640 ($20^{\circ}C$, Verschuereen 1983)

102125, 120220 ($20.7^{\circ}C$, quoted exptl., interpolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 7.14122 - 1606.85/(292.482 + t/^{\circ}C)$, temp range: -0.2 to $34.3^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

120230 (calculated-Antoine eq., Dean 1985, 1992)

$\log (P/mmHg) = 8.00552 - 1600.017/(291.809 + t/^{\circ}C)$, temp range: liquid (Antoine eq., Dean 1985, 1992)

121300 (selected, Riddick et al. 1986)

$\log (P/kPa) = 6.1814 - 1070.6/(236.0 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

120700 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.1410 - 1034.5/(-43.15 + T/K)$; temp range 272 – $294 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.03292 - 1012.828/(-41.823 + T/K)$; temp range 293 – $377 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P/mmHg) = 87.3702 - 3.6822 \times 10^3/(T/K) - 31.548 \cdot \log (T/K) + 2.0114 \times 10^{-2} \cdot (T/K) + 5.5341 \times 10^{-13} \cdot (T/K)^2$; temp range 150 – $461 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 6.692 (shake flask-concentration ratio-GC, Buttery et al. 1969)
- 8.924 (calculated K_{AW} s, Buttery et al. 1969)
- 6.672 (exptl., Hine & Mookerjee 1975)
- 5.946, 5.423 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
- 1.336, 8.0 (0, 25°C, gas stripping-GC, Snider & Dawson 1985)
- 6.75 (review, Gaffney et al. 1987)
- 2.578* (gas stripping-headspace GC, measured range 15–35°C, Betterton & Hoffmann 1988)
- 6.80* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
- $\ln [K_{\text{H}}'/(M/\text{atm})] = -6.03 + 276/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
- $\ln [K_{\text{H}}'/(M/\text{atm})] = -5.21 + 1984/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity $35 \pm 1\text{‰}$), Zhou & Mopper 1990)
- 10.18 (calculated-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
- 5.47* (20°C, headspace-GC, measured range 10–40°C, Benkelberg et al. 1995)
- 8.72* (headspace-GC, artificial seawater, measured range 16–40°C, Benkelberg et al. 1995)
- $\ln (k_{\text{H}}/\text{atm}) = (20.4 \pm 0.1) - (5671 \pm 22)/(T/K)$; temp range 10–40°C (headspace-GC measurements, Benkelberg et al. 1995)
- 5.14 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
- 6.33 (solid-phase microextraction SPME-GC, Bartelt 1997)
- 6.69 (equilibrium headspace-GC, Marin et al. 1999)
- 5.39 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
- $\log K_{\text{AW}} = 5.324 - 2340/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.52 (generator column-HPLC, Wasik et al. 1981)
- 0.36 (generator column-GC, Tewari et al. 1982)
- 0.43 (calculated, Verschueren 1983)
- 0.45 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 2.3.0 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986);
calculated lifetime of 6 d (Atkinson 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and or Arrhenius equation see reference:

$k_{\text{OH}} = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

$k_{\text{OH}} = 1.6.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (long-path Fourier transform IR, Niki et al. 1978)

$k = 0.1 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by RO_2 radical at 30°C in aquatic systems with half-life of $8 \times 10^4 \text{ d}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen at 25°C in aquatic systems with half-life $> 00 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}} = (12.8 \pm 4.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k = (1.5 \pm 0.2) \text{ M}^{-1} \cdot \text{s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}} = (12.2 \pm 2.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Semmes et al. 1985; quoted, Atkinson 1985)

$k_{\text{O}_3} = (3.4 \pm 0.5) \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (Stedman & Niki 1973; quoted, Atkinson & Carter 1984)

$k_{\text{OH}} = 9.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k_{\text{O}_3} \leq 6 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $296 \pm 2 \text{ K}$ (Atkinson et al. 1981, 1982; quoted, Atkinson & Carter 1984; Atkinson 1985)

$k_{\text{HO}_2} = 1.0 \times 10^{-17} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ for the gas-phase reaction with HO_2 radical at 293 K in the atmosphere (Barnes et al. 1982; quoted, Carlier et al. 1986)

$k_{\text{OH}} = 1.62 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$; and $k_{\text{NO}_3} = 3.02 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K in air (Atkinson et al. 1984)

$k_{\text{NO}_3} = 1.40 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $298 \pm 1 \text{ K}$ (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = 1.60 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Baulch et al. 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = (14.7 \pm 2.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Michael et al. 1985; quoted, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 1.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.62 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}} = 1.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.7 d^{-1} , $k_{\text{O}_3} \leq 6.0 \times 10^{-21} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a loss rate of $\leq 0.0004 \text{ d}^{-1}$, $k_{\text{NO}_3} = 2.5 \times 10^{-15} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ with a loss rate of 0.05 d^{-1} (review, Atkinson 1985)

$k_{\text{OH}}^* = 1.53 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = 16.22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 3.02 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Sabljić & Güsten 1990; Müller & Klein 1991)

$k_{\text{NO}_3} = 2.78 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1991)

$k_{\text{OH}} = 10.64 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} < 0.24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);
atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994);
calculated lifetimes of 8.8 h, 17 d and $> 4.5 \text{ yr}$ for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.2.1

Reported vapor pressures of ethanal (acetaldehyde) at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Coles & Popper 1950	
summary of literature data		isoteniscope method	
t/°C	P/Pa	t/°C	P/Pa
-81.5	133.3	-0.20	44263
-65.1	666.6	2.70	49996
-56.8	1333	6.70	59062
-47.8	2666	9.30	65861
-37.8	5333	11.6	70794
-31.4	7999	15.3	76927
-22.6	13332	17.6	90926
-10.0	26664	20.7	102125
4.90	53329	30.8	149321
20.2	101325	34.4	167852
mp/°C	-123.5	bp/°C	20.4
		eq. 1	P/mmHg
		A	7.694
		B	1413

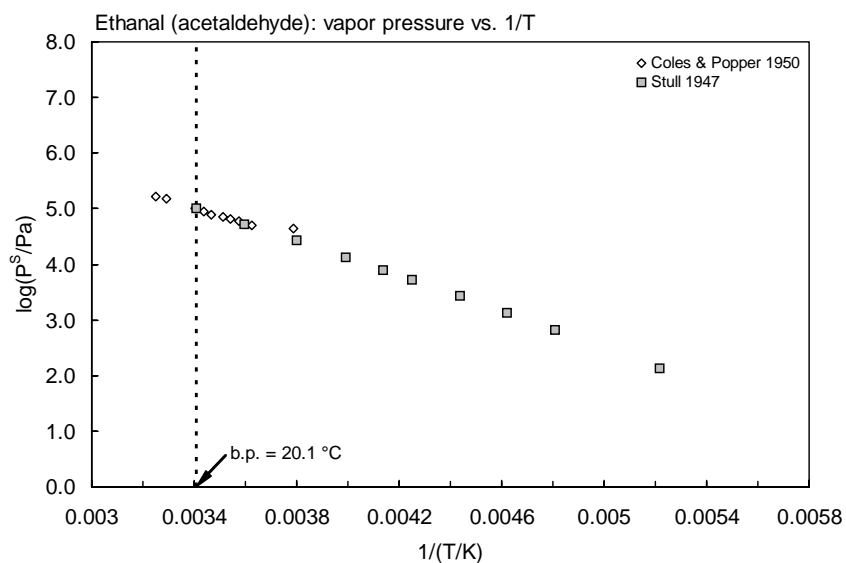


FIGURE 12.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethanal.

TABLE 12.1.1.2.2

Reported Henry's law constants of ethanal (acetaldehyde) at various temperatures and temperature dependence equations

$$\begin{aligned}\ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) & (4a) \\ K_{AW} &= A - B\cdot(T/K) + C\cdot(T/K)^2 & (5) & & \end{aligned}$$

1.

Snider & Dawson 1985		Betterton & Hoffmann 1988		Zhou & Mopper 1990			
gas stripping-GC		gas stripping-GC, spec.		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
				fresh water		sea water	
0	1.336	5	1.829	10	2.277	10	3.147
25	8.00	10	2.578	17	-	17	5.170
		25	8.888	25	6.80	25	7.735
enthalpy of transfer:		35	15.446	30	8.238	30	9.296
$\Delta H/(\text{kJ mol}^{-1}) = -46.024$		$\Delta H/(\text{kJ mol}^{-1}) = -52.1$		35	10.55	35	11.78
		at 25°C		40	-	40	14.90
				45	15.59	45	17.78
				eq. 1a	$K_H'/(M/\text{atm})$	eq. 1a	$K_H'/(M/\text{atm})$
				A	-6.03	A	-5.21
				B	-2164	B	-1894

2.

Benkelberg et al. 1995			
equilibrium vapor phase concentration-headspace GC			
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
deionized water		artificial sea water	
10	2.754	16	5.070
15	3.940	25	8.718
20	5.472	30	11.69
30	10.268	40	19.716
40	18.968		
for deionized and rain water:			
eq. 3	k_H/atm		
A	20.4 ± 0.1		
B	5671 ± 22		
$\Delta H/(\text{kJ mol}^{-1}) = -47.15$			

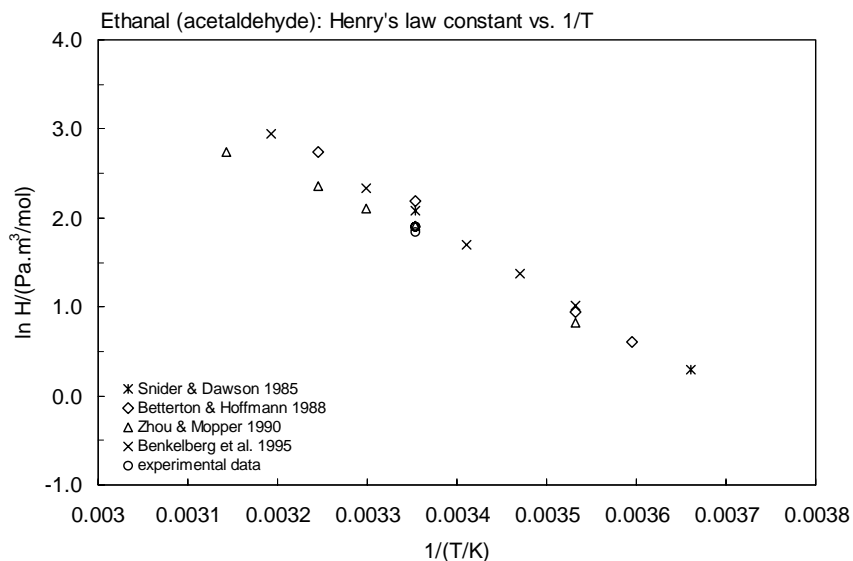
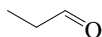


FIGURE 12.1.1.2.2 Logarithm of Henry's law constant versus reciprocal temperature for ethanal.

12.1.1.3 Propanal (Propionaldehyde)



Common Name: Propionaldehyde

Synonym: propanal

Chemical Name: propionaldehyde, propanal

CAS Registry No: 123-38-6

Molecular Formula: C_3H_6O , CH_3CH_2CHO

Molecular Weight: 58.079

Melting Point ($^{\circ}C$):

-80 (Lide 2003)

Boiling Point ($^{\circ}C$):

48 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8058 (Weast 1982–83)

0.7970 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

72.9 (calculated-density, Stephenson & Malanowski 1987)

74.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Fusion ΔH_{fus} (kJ/mol):Entropy of Fusion ΔS_{fus} (J/mol K):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

160000 ($20^{\circ}C$, Seidell 1941)200000 ($20^{\circ}C$, Verschueren 1983)

306000 (Dean 1985; Riddick et al. 1986)

405000 (selected, Yaws et al. 1990)

310000*, 269000 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 12.3 – $50^{\circ}C$, Stephenson 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

67661* ($39.07^{\circ}C$, ebulliometry, measured range 39.07 – $50.29^{\circ}C$, Dreisbach & Shrader 1949) $\log(P/mmHg) = 7.08683 - 1178.9/(230 + t/^{\circ}C)$; temp range not specified (Antoine eq., Dreisbach & Martin 1949)42300* ($23^{\circ}C$, measured range 13.1 – $48.06^{\circ}C$, Ambrose & Sprake 1974)

42340 (interpolated-Antoine eq., Boublik et al. 1984)

 $\log(P/kPa) = 6.2902 - 1210.87/(234.65 + t/^{\circ}C)$, temp range 13.1 – $48.06^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose & Sprake 1974, Boublik et al. 1984)

42490, 42360 (interpolated-Antoine eq. I and II, Stephenson & Malanowski 1987)

 $\log(P_L/kPa) = 6.2047 - 1166.99/(-43.15 + T/K)$; temp range 290–322 K (Antoine eq.-I, Stephenson & Malanowski 1987) $\log(P_L/kPa) = 6.2336 - 1180/(-42.0 + T/K)$; temp range 250–330 K (Antoine eq.-II, Stephenson & Malanowski 1987)

23190 (calculated-solvatochromic parameters, Banerjee et al. 1990)

 $\log(P/mmHg) = 26.1637 - 2.3059 \times 10^3/(T/K) - 6.5289 \cdot \log(T/K) - 2.3065 \times 10^{-10} \cdot (T/K) + 2.5454 \times 10^{-6} \cdot (T/K)^2$; temp range 193–496 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

7.436 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

7.486 (exptl., Hine & Mookerjee 1975)

- 8.40, 8.21 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 8.305* (gas stripping-HPLC/UV, measured range 10–45°C, Zhou & Mopper 1990)
 $\ln [K_H'/(M/atm)] = -7.15 + 2467/(T/K)$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
 $\ln [K_H'/(M/atm)] = -6.60 + 2273/(T/K)$, temp range 25–35°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)
 7.486, 13.62 (quoted, correlated-molecular structure, Russell et al. 1992)
 5.48 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)
 $\log K_{AW} = 5.324 - 2237/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.83 (calculated, Verschueren 1983)
 0.59 (shake flask, Log P Database, Hansch & Leo 1987)
 0.59 (recommended, Sangster 1989)
 0.59 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 3.02 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 3.2 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 3.06 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (discharge flow system-MS, Morris & Niki 1971)

photooxidation $t_{1/2} < 0.24 \text{ h}$ for the gas-phase reaction with OH radicals in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = 2.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (long-path Fourier transform IR, Niki et al. 1978)

$k_{OH} = (18.5 \pm 2.1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Audley et al. 1981; quoted, Atkinson 1985),

$k_{OH} = (19.5 \pm 1.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k = (2.5 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = 1.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (review, Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{OH} = (17.1 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Semmes et al. 1985; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 2.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 3.3\text{--}33 \text{ h}$ in air, based on measured reaction rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991)

$k_{OH} = 1.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 16.55 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: biodegradation rate constants $k = 0.046\text{--}0.063 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b); aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on aerobic biological screening test data (Gerhold & Malaney 1966; Dore et al. 1975; Urano & Kato 1986; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} < 0.24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2}$ = 3.3–33 h in air, based on measured reaction rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).
Surface water: $t_{1/2}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Ground water: $t_{1/2}$ = 48–336 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Sediment:
Soil: $t_{1/2}$ = 24–168 h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).
Biota:

TABLE 12.1.1.3.1
Reported aqueous solubilities and vapor pressures of propanal (propionaldehyde) at various temperatures

Aqueous solubility		Vapor pressure					
Stephenson 1993		Dreisbach & Shrader 1949		Dreisbach & Martin 1949		Ambrose & Sprake 1974	
shake flask-GC/TC		ebulliometry		ebulliometry		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
12.3	477000	39.07	67661	data presented in		13.1	25300
15.6	368000	50.29	101325	log P = A – B/(C + t/°C)		23.0	42300
20.0	310000			eq. 2	P/mmHg	29.5	51000
30.0	269000			A	7.08683	47.95	101300
40.0	235000			B	1178.9	48.06	101700
50.0	197000			C	230		
				bp/°C	50.29		

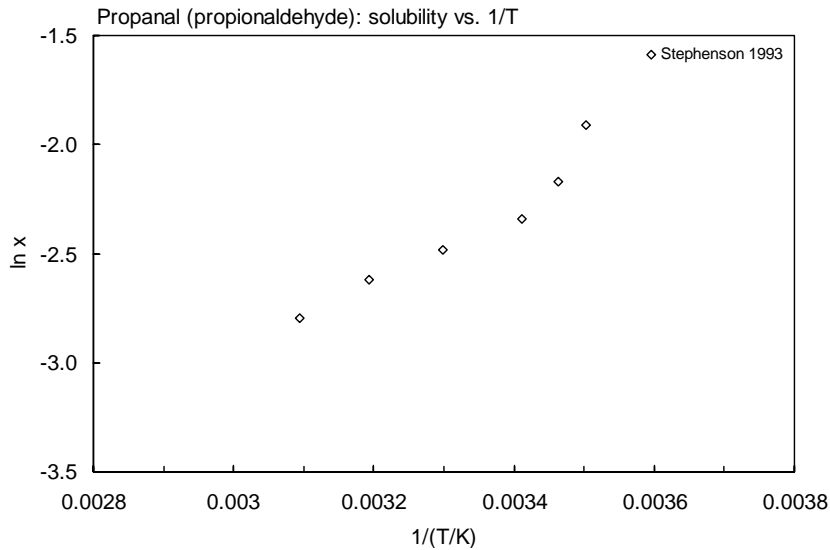


FIGURE 12.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for propanal.

TABLE 12.1.1.3.2

Reported Henry's law constants of propanal (propionaldehyde) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Zhou & Mopper 1990

gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
fresh water		sea water	
10	2.605	10	3.389
17	-	17	6.495
25	8.305	25	10.13
30	10.67	30	12.67
35	14.07	35	16.34
40	-	40	22.03
45	23.56	45	28.15
eq. 1a	$K_H'/(M/\text{atm})$	eq. 1a	$K_H'/(M/\text{atm})$
A	-7.15	A	-6.60
B	-2467	B	-2273

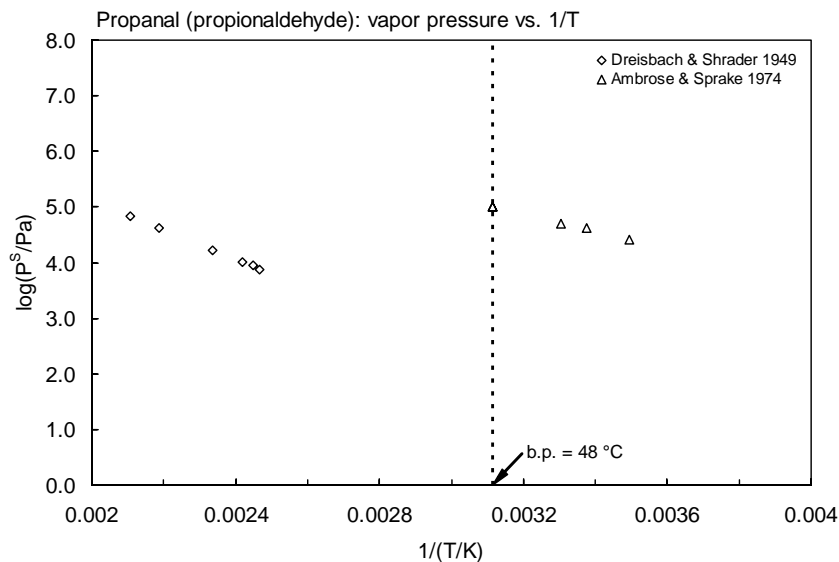


FIGURE 12.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for propanal.

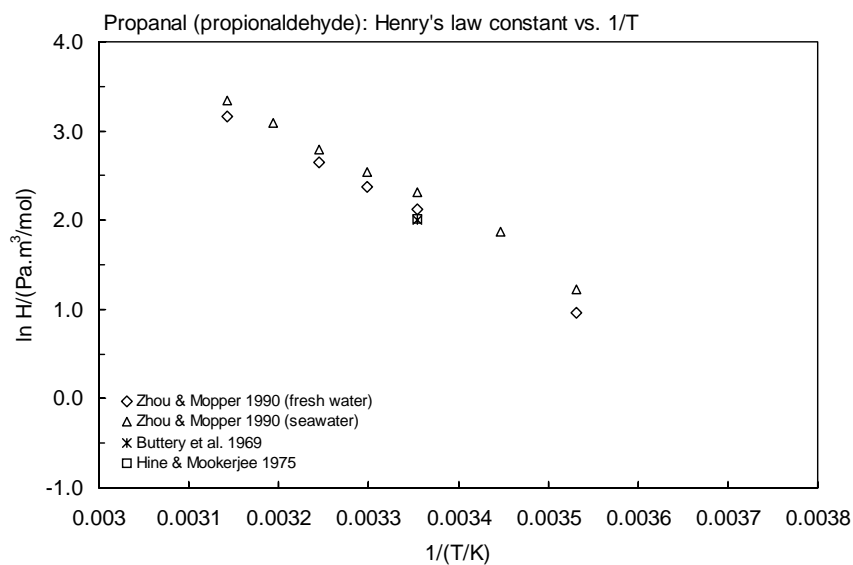
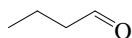


FIGURE 12.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for propanal.

12.1.1.4 Butanal (*n*-Butyraldehyde)

Common Name: *n*-Butyraldehyde

Synonym: 1-butanal, butylaldehyde, butyric aldehyde

Chemical Name: butyraldehyde, butanal

CAS Registry No: 123-72-8

Molecular Formula: C_4H_8O , $CH_3CH_2CH_2CHO$

Molecular Weight: 72.106

Melting Point ($^{\circ}C$):

−96.86 (Lide 2003)

Boiling Point ($^{\circ}C$):

74.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8170 (Weast 1982–83; Verschueren 1983)

0.8016 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

90.0 ($20^{\circ}C$, calculated-density)

96.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

11.088 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

36000 ($20^{\circ}C$, quoted, Palit 1947)

37840 (Deno & Berkheimer 1960)

37000, 71000 (lit. values, Verschueren 1983)

71000 (Dean 1985; Riddick et al. 1986)

83700 (selected, Yaws et al. 1990)

74400*, 54800 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $70^{\circ}C$, Stephenson 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19372* ($30.71^{\circ}C$, measured range 30.71 – $74.03^{\circ}C$, Seprakova et al. 1959; quoted, Boublik et al. 1984)

9464 ($20^{\circ}C$, Verschueren 1983)

14798 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.52728 - 921.802/(186.564 + t/^{\circ}C)$; temp range 30.71 – $74.03^{\circ}C$ (Antoine eq. from reported exptl. data of Seprakova et al. 1959, Boublik et al. 1984)

14785 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.91048 - 946.35/(246.68 + t/^{\circ}C)$; temp range -87 to $7^{\circ}C$ (Antoine eq., Dean 1985, 1992)

15700 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.1461 - 1233.0/(223.0 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

14780 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.68618 - 994.1/(-78.05 + T/K)$; temp range 293 – 349 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.40874 - 1182.472/(T/K)$; temp range 348 – 423 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 66.8411 - 3.6784 \times 10^3/(T/K) - 22.609 \cdot \log(T/K) + 1.1697 \times 10^{-2} \cdot (T/K) + 2.9647 \times 10^{-13} \cdot (T/K)^2$; temp range 177 – 525 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11.65 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)

11.59, 11.594, 12.14 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

11.65 (gas stripping-HPLC, Zhou & Mopper 1990)

3.237, 11.65, 15.59, 20.68, 36.19 (10, 25, 30, 35, 45°C, gas-stripping-HPLC-UV, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -8.07 + 2701/(T/K)$; temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -8.20 + 2698/(T/K)$; temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)

11.59, 11.59 (quoted, correlated-molecular structure, Russell et al. 1992)

7.26 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 6.244 - 2571/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.20 (Hansch & Leo 1979)

0.88 (shake flask, Log P Database, Hansch & Leo 1987)

0.88 (recommended, Sangster 1989)

0.88 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.39 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: rate constant $k = 2.7 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

photooxidation $t_{1/2} = 114 \text{ d}$ to 19 yr in water, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991)

$k_{OH} = (26.2 \pm 3.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Audley et al. 1981; quoted, Atkinson 1985)

$k_{OH} = (25.3 \pm 0.6) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate method, Kerr & Sheppard 1981; quoted, Atkinson 1985)

$k_{OH} = 25 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k = (2.5 \pm 0.4) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 2.0–6.0 and 20–23°C (Hoigné & Bader 1983)

$k_{OH} = (30.8 \pm 4.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence technique. Semmes et al. 1985; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 2.55 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 2.8\text{--}28 \text{ h}$ in air, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991)

$k_{OH}^* = 2.35 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis:

Biodegradation: rate constants $k = 0.044\text{--}0.069 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b);

aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on aerobic biological screening test data (Lamb & Jenkins 1952; Heukelekian & Rand 1955; Dore et al. 1975; Urano & Kato 1986b; selected, Howard et al. 1991);
 aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.8\text{--}28$ h, based on measured rate constant for the gas-phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);
 calculated lifetimes of 5.9 d for reaction with OH radical (Atkinson 2000).

Surface water: photooxidation $t_{1/2} = 114$ d to 19 yr, based on measured rate constant for the reaction with OH radical in water (Anbar & Neta 1967; Dorfman & Adams 1973; selected, Howard et al. 1991);
 $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.1.4.1

Reported aqueous solubilities and vapor pressures of butanal (*n*-butyraldehyde) at various temperatures

Aqueous solubility		Vapor pressure	
Stephenson 1993		Seprakova et al. 1959	
shake flask-GC/TC		in Boublik et al. 1984	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
0	118200	30.71	19372
10.0	91200	38.36	26771
20.0	74400	43.93	33584
30.0	54800	48.33	39997
40.0	47100	52.36	46663
50.0	42500	55.90	53329
60.0	41700	62.29	66661
70.0	38900	67.73	79993
		74.03	97512
bp/ $^{\circ}\text{C}$	75		
eq in Boublik et al. 1984			
$\log P = A - B/(C + t/^{\circ}\text{C})$			
eq. 2			
		P/kPa	
		A	5.52728
		B	921.802
		C	186.564
		bp/ $^{\circ}\text{C}$	75.195

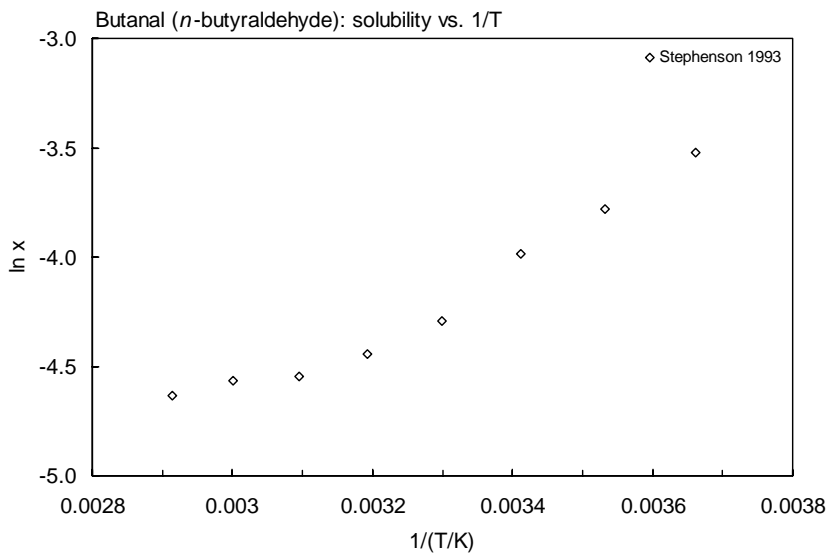


FIGURE 12.1.1.4.1 Logarithm of mole fraction solubility (ln *x*) versus reciprocal temperature for butanal.

TABLE 12.1.1.4.2
Reported Henry’s law constants of butanal (*n*-butyraldehyde) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$	(5)		

Zhou & Mopper 1990

gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
fresh water		sea water	
10	3.237	10	4.312
17	-	17	8.660
25	11.65	25	16.08
30	15.83	30	20.68
35	20.68	35	28.15
40	-	40	38.97
45	36.18	45	50.66
eq. 1a	$K_H'/(M/\text{atm})$	eq. 1a	$K_H'/(M/\text{atm})$
A	-8.07	A	-8.20
B	-2704	B	-2698

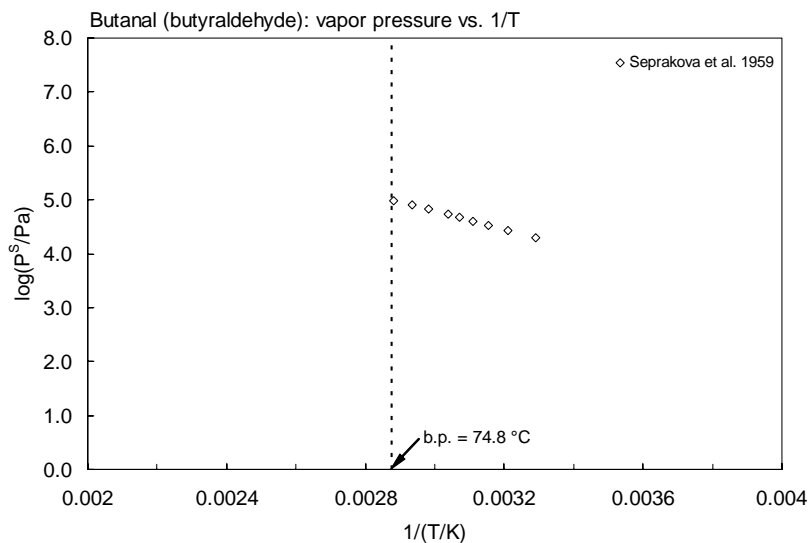


FIGURE 12.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for butanal.

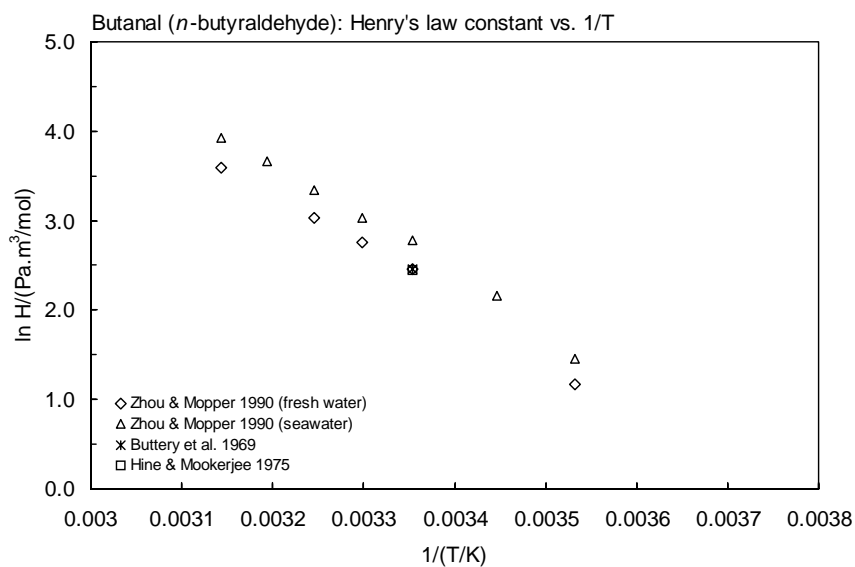
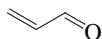


FIGURE 12.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for butanal.

12.1.1.5 2-Propenal (Acrolein)



Common Name: Acrolein

Synonym: 2-propenal, acraldehyde, acrylic aldehyde, allylaldehyde, acrylaldehyde, aqualin

Chemical Name: 2-propenal

CAS Registry No: 107-02-8

Molecular Formula: C_3H_4O , $CH_2=CHCHO$

Molecular Weight: 56.063

Melting Point ($^{\circ}C$):

−87.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

52.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8389 (Riddick et al. 1986)

Dissociation Constant:

Molar Volume (cm^3/mol):

66.8 ($20^{\circ}C$, calculated-density)

66.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

208000 ($20^{\circ}C$, Günther et al. 1968; Callahan et al. 1979; Verschueren 1977, 1983)

102020 (shake flask-radioactive analysis, Veith et al. 1980)

208000 (selected, Riddick et al. 1986)

229000*, 230000 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range $0-53^{\circ}C$, Stephenson 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

26664* ($17.5^{\circ}C$, summary of literature data, temp range -64.5 to $52.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 7628.8/(T/K)] + 8.033866$; temp range: -64.5 to $52.5^{\circ}C$, (Antoine eq., Weast 1972–73)

29330, 44000 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1977, 1983)

35300 (Riddick et al. 1986, Howard 1989)

36610, 35360 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.19181 - 1204.95/(-37.8 + T/K)$; temp range 208–326 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2878 - 1231.003/(-38.405 + T/K)$; temp range 250–306 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 57.9815 - 3.0933 \times 10^3/(T/K) - 19.638 \cdot \log(T/K) + 1.1486 \times 10^{-2} \cdot (T/K) - 2.3854 \times 10^{-14} \cdot (T/K)^2$; temp range 185–506 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

2.84, 13.77 (0 , $25^{\circ}C$, headspace-GC, Snider & Dawson 1985)

12.36 (review, Gaffney et al. 1987)

0.446 (Howard 1989)

5.48 ($20^{\circ}C$, selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.823 - 2110/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.09 (quoted, Callahan et al. 1979)

0.90 (measured value, Veith et al. 1980)

- 0.10 (shake flask, Log P Database, Hansch & Leo 1987; recommended, Sangster 1993)
 –0.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 2.54 (bluegill sunfish, Barrows et al. 1980)
 2.54 (bluegill sunfish, Veith et al. 1980)
 –0.22 (estimated- K_{OW} , Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.38 (estimated- K_{OW} , Howard et al. 1989)
 –0.219 (calculated- K_{OW} , Kolliig 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 10$ d from a model river (Howard 1989);

Photolysis: $t_{1/2} = 3.5$ d, based on measured quantum yields (Howard 1989).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{O_3} = 6.4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson & Carter 1984)

$k_{OH} = (1.90 - 2.53) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in air (Atkinson 1985)

$k_{OH} = 20.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 23.5°C using propylene as reference compound, with a atmospheric lifetime of 0.56 d (Edney et al. 1986)

$k_{NO_3} = 5.9 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a calculated atmospheric lifetime of 16 d, $k_{OH} = 2.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 1.2 d; and $k_{O_3} = 2.8 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with a lifetime of 59 d at room temp. (Atkinson et al. 1987)

$k_{OH}(\text{calc}) = 2.29 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.96 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH} = 1.99 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

atmospheric $t_{1/2} = 3.4\text{--}33.7$ h, based on rate constant for reaction with OH radical (Howard et al. 1991)

$k_{OH} = 22.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{NO_3} = 1.15 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ((Sabljić & Güsten 1990; Müller & Klein 1991)

$k_{OH}(\text{calc}) = 17.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: no hydrolyzable groups (Callahan et al. 1979).

Biodegradation: $t_{1/2} = 29$ h (natural unsterilized water) and $t_{1/2} = 43$ h in sterilized (thymol-treated) water (Bowmer & Higgins 1976, quoted, Howard 1989);

aqueous aerobic $t_{1/2} = 168\text{--}672$ h, based on acclimated aqueous screening test data; and aqueous anaerobic $t_{1/2} = 672\text{--}2880$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation: $t_{1/2} < 4$ d (Callahan et al. 1979)

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: atmospheric lifetime of 0.56 d due to reaction with OH radical (Edney et al. 1986);

calculated atmospheric lifetimes: 16 d for reaction with NO_3 radical, 1.2 d with OH radical and 59 d with O_3 (Atkinson et al. 1987);

$t_{1/2} = 10\text{--}13$ h for reaction with photochemically generated hydroxyl radical, $t_{1/2} = 18$ d for reaction with ozone and $t_{1/2} = 3.5$ d for photodissociation in the atmosphere (Howard 1989);

$t_{1/2} = 3.4\text{--}33.7$ h, based on photooxidation half-life in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: removal $t_{1/2} = 2.0$ to 2.5 d from water (Howard 1989);

First order $k = 0.163 \text{ h}^{-1}$ in 8 agricultural canals and varies between 0.104 and 0.211 h^{-1} at pH 7.1 to 7.5 and water temperature of 16–24°C, the mean value corresponds to $t_{1/2} = 4.25$ h at 21°C (Bowmer & Sainty 1977)

$t_{1/2} \sim 8$ and 23 d for reacting with singlet oxygen and alkylperoxy radicals in natural sunlit water (estimated, Howard 1989),

aqueous aerobic $t_{1/2}$ = 168–672 h, based on acclimated aqueous screening test data; and aqueous anaerobic $t_{1/2}$ = 672–2880 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991)

$k = 0.015 \text{ h}^{-1}$ at 21°C and pH 7.0, corresponding to $t_{1/2} = 46 \text{ h}$ in dilute buffered solutions of acrolein in distilled water. (Nordone et al. 1996)

Dissipation $k = 0.068 \text{ h}^{-1}$ with $t_{1/2} = 10.2 \text{ h}$ and $k = 0.028 \text{ h}^{-1}$ with $t_{1/2} = 7.3 \text{ h}$ in weedy (Pump Canal, 12–20°C) and non-weedy agricultural canals (Lateral 1, 12–18°C), respectively, dissipation is the result of numerous processes including degradation, volatilization, adsorption and dilution (Nordone et al. 1996)

Ground water: $t_{1/2} = 336$ –1344 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168$ –672 h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.1.5.1

Reported aqueous solubilities and vapor pressures of 2-propenal(acrolein) at various temperatures

Aqueous solubility		Vapor pressure	
Stephenson 1993		Stull 1947	
shake flask-GC/TC		summary of literature data	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
0	197000	–64.5	133.3
10.0	209000	–46.0	666.6
20.0	229000	–36.7	1333
30.0	230000	–26.3	2666
40.0	242000	–15.0	5333
53.0	245000	–7.5	7999
		2.5	13332
		17.5	26664
		34.5	53329
		52.5	101325
		mp/ $^{\circ}\text{C}$	–87.7

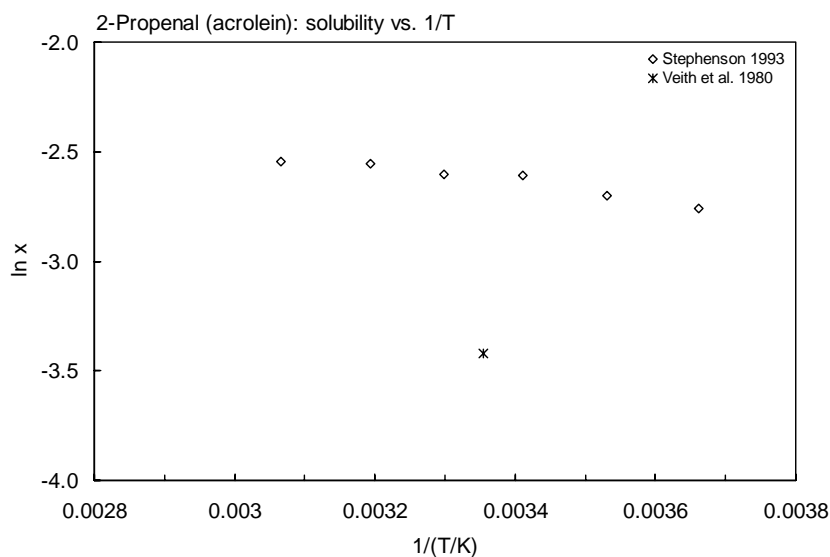


FIGURE 12.1.1.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-propenal.

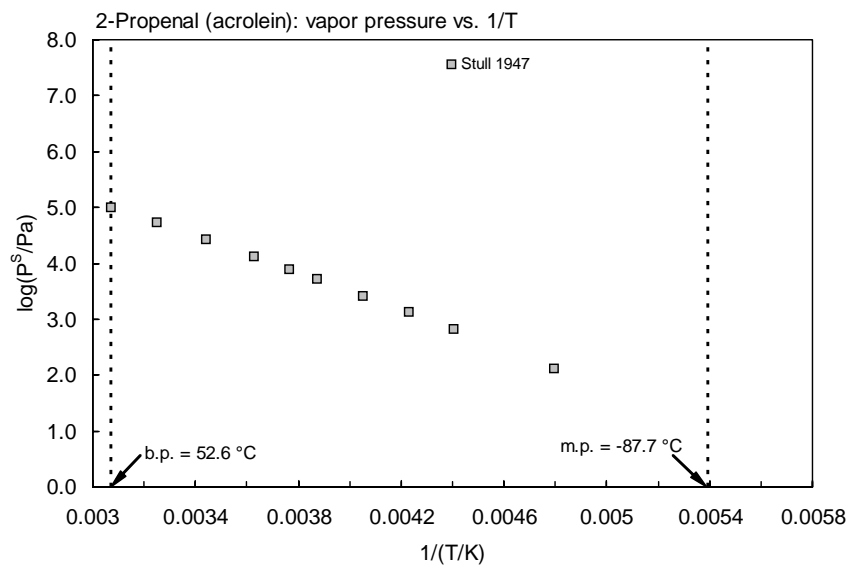
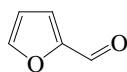


FIGURE 12.1.1.5.2 Logarithm of vapor pressure versus reciprocal temperature for 2-propenal.

12.1.1.6 Furfural (2-Furaldehyde)



Common Name: Furfural

Synonym: 2-furaldehyde, 2-furancarboxaldehyde; furfurole, 2-furancarbal, fural, furfuraldehyde, furole

Chemical Name: furfural

CAS Registry No: 98-01-1

Molecular Formula: C₅H₄O₂

Molecular Weight: 96.085

Melting Point (°C):

−38.1 (Lide 2003)

Boiling Point (°C):

161.7 (Lide 2003)

Density (g/cm³ at 20°C):

1.16 (Verschueren 1983)

Dissociation Constant:

Molar Volume (cm³/mol):

82.9 (calculated-density, Stephenson & Malanowski 1987)

92.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

82000 (40°C, synthetic method, Jones 1929)

91593 (shake flask-volumetric method, Booth & Everson 1948)

92900 (26.7°C, shake flask-turbidity, Skrzec & Murphy 1954)

77830 (generator column-HPLC/UV, Tewari et al. 1982)

79400*, 84000 (20°C, 30°C, shake flask-GC/TC, measured range 0–90°C, Stephenson 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1066.6* (39.9°C, ebulliometry, measured range 40–170.6°C, Evans & Aylesworth 1926)

220.4* (interpolated-regression of tabulated data, temp range 18.5–161.8°C, Stull 1947)

1767* (55.67°C, Ramsay-Young method, measured range 55.6–170°C, Matthews et al. 1950)

log (P/mmHg) = A – B/(T/K) – C log (T/K); temp range 55.6–170°C (Kirchhoff eq., Matthews et al. 1950)

log (P/mmHg) = [−0.2185 × 11614.6/(T/K)] + 8.729884; temp range 18.5–161.8°C (Antoine eq., Weast 1972–73)

133.3, 400 (20°C, 30°C, Verschueren 1983)

log (P/kPa) = 5.62941 – 1124.583/(148.829 + t/°C), temp range 92.3–170.6°C (Antoine eq. derived from Evans & Aylesworth 1926 data, Boublik et al. 1984)

log (P/kPa) = 5.76606 – 1236.745/(167.368 + t/°C), temp range 55.87–160.8°C (Antoine eq. derived from Matthews et al. 1950 data, Boublik et al. 1984)

208.0 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 6.91048 – 946.35/(246.68 + t/°C), temp range −87 to 7°C (Antoine eq., Dean 1985, 1992)

333.3 (Riddick et al. 1986)

313.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

log (P₁/kPa) = 6.41784 – 1663.16/(−57.88 + T/K), temp range 357–435 K (Antoine eq., Stephenson & Malanowski 1987)

log (P/mmHg) = 32.0337 – 3.3161 × 10³/(T/K) + 10.171·log (T/K) – 2.1115 × 10^{−2}·(T/K) + 9.2045 × 10^{−6}·(T/K)²; temp range 237–657 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa·m³/mol):

0.375 (calculated-P/C, Howard 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.34	(20°C, shake flask, Korenman 1972)
0.52	(generator column-HPLC/UV, Tewari et al. 1982)
0.41, 0.52	(shake flask, Log P Database, Hansch & Leo 1987)
0.46	(recommended, Sangster 1993)
0.41	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

0.079	(estimated- K_{ow} , Lyman et al. 1982; quoted, Howard 1993)
-2.097	(estimated-S, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

1.602	(soil, estimated- K_{ow} , Lyman et al. 1982; quoted, Howard 1993)
0.00	(soil, estimated-S, Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: based on calculated Henry's law constant, the estimated $t_{1/2} \sim 9.9$ d from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation 41.0 mg COD $g^{-1} h^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: estimated photooxidation $t_{1/2} \sim 0.44$ d for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard 1993).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.6.1
Reported aqueous solubilities of furfural (2-furaldehyde) at various temperatures

Stephenson 1993

shake flask-GC/TC	
t/°C	S/g·m⁻³
0	82200
10.0	78600
20.0	79400
30.0	84000
40.0	89400
50.0	95000
60.0	102800
70.0	109700
80.0	125600
90.0	147400

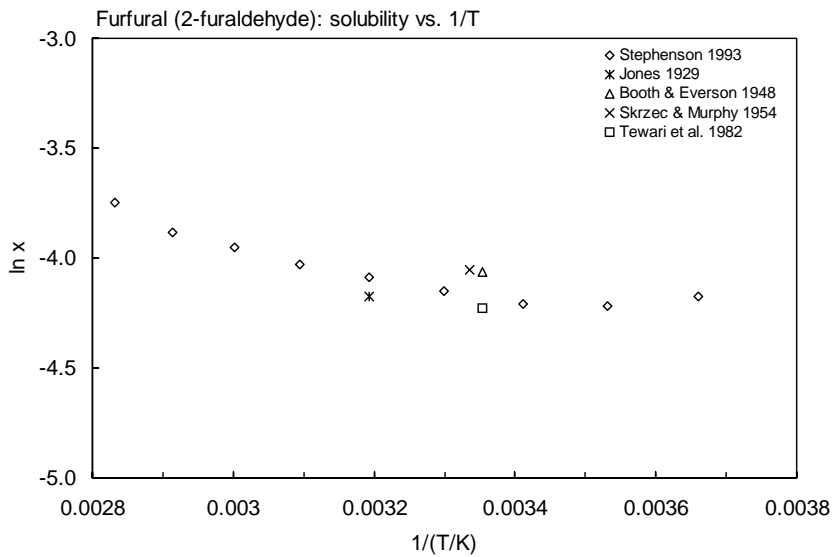


FIGURE 12.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for furfural.

TABLE 12.1.1.6.2
Reported vapor pressures of furfural (2-furaldehyde) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Evans & Aylesworth 1926		Stull 1947		Matthews et al. 1950			
ebulliometry		summary of literature data		Ramsay-Young method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
92.30	9199	18.5	133.3	55.67	1767	continued	
120.3	28531	42.6	666.6	56.07	1793	139.95	56368
131.6	41330	54.8	1333	64.50	2786	143.8	61635
140.2	54795	67.8	2666	67.70	3321	146.85	69034
154.4	83326	82.1	5333	75.05	4600	149.65	71727
159.0	94259	91.5	7999	76.47	5034	151.70	77247
160.9	99192	103.4	13332	84.95	7254	153.95	82473
163.8	108257	121.8	26664	87.38	8239	155.10	85459
170.6	128789	141.8	53329	92.15	9959	160.75	101885
		161.8	101325	93.05	10308	bp/K	433.8
				96.77	12060	$\Delta H_v/(\text{kJ mol}^{-1}) = 38.59$ at bp	
		mp/°C	−35.6	102.13	15079	Kirchhoff, Rakine, Dupre eq.	
				103.31	15705	eq. 4	P/mmHg
				103.09	17012	A	29.3205
				107.27	18292	B	3530.52
				111.65	21651	C	6.9418
				116.25	24731		
				118.40	27184		
				120.85	29744		
				124.75	34144		

(Continued)

TABLE 12.1.1.6.2 (Continued)

Evans & Aylesworth 1926		Stull 1947		Matthews et al. 1950			
ebulliometry		summary of literature data		Ramsay-Young method			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				126.05	35064		
				126.35	35130		
				132.15	43583		
				133.80	45303		
				135.95	48942		
				138.35	53262		

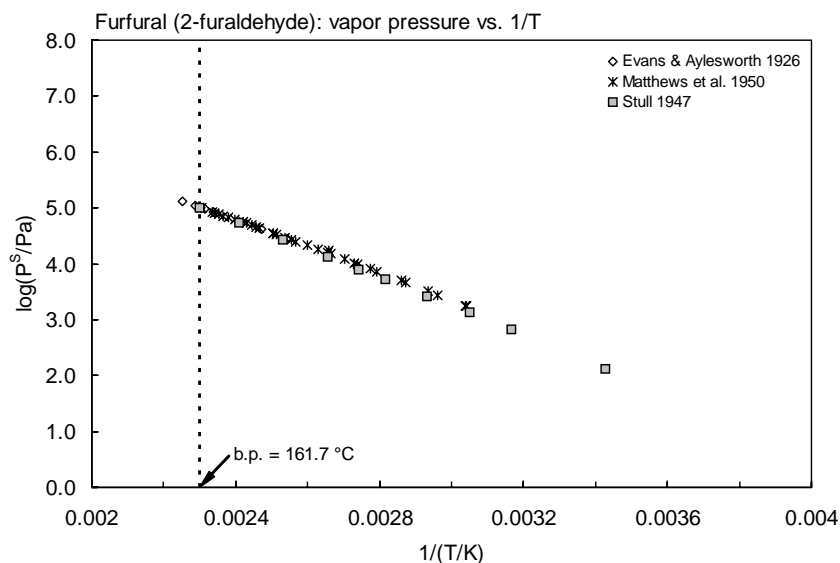
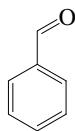


FIGURE 12.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for furfural.

12.1.1.7 Benzaldehyde



Common Name: Benzaldehyde

Synonym: benzenecarbonal, oil of bitter almonds

Chemical Name: benzaldehyde

CAS Registry No: 100-52-7

Molecular Formula: C_7H_6O , C_6H_5CHO

Molecular Weight: 106.122

Melting Point ($^{\circ}C$):

-57.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

178.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0401 (24.94 $^{\circ}C$, measured, Ambrose et al. 1975)

1.0447 (Dean 1985)

1.0446 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

102.0 (calculated-density, Chiou 1985)

118.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

9.322 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} J/mol K:

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

2991 (quoted, Deno & Berkheimer 1960)

2857 (1 in 350 parts, Merck Index 1960)

3490, 3500 (quoted Ph. D. theses from University of London, Mitchell et al. 1964)

6550, 6580 (shake flask-gravimetric method, shake flask-GC/FID, Mitchell et al. 1964)

6900–7000 (shake flask-refractive index method, Carless & Swarbrick 1964)

7200 ($20^{\circ}C$, shake flask-GC, Tewari et al. 1982)

3000 (20 – $25^{\circ}C$, shake flask-GC, Urano et al. 1982)

3300 (Verschuereen 1983)

3279 (shake flask-GC, Chiou 1985)

3000 ($20^{\circ}C$, Riddick et al. 1986)

7200*, 7400 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90^{\circ}C$, Stephenson 1993)

3514 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3*, 145.2 ($26.2^{\circ}C$, extrapolated-regression of tabulated data, temp range 26.2 – $179^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11657.8/(T/K)] + 8.580362$; temp range 26.2 – $179^{\circ}C$ (Antoine eq., Weast 1972–73)

137.0* (ebulliometry-extrapolated from Antoine eq., measured range 38.5 – $89.3^{\circ}C$, Ambrose et al. 1975b)

$\log(P/kPa) = 6.20251 - 1611.217/(T/K - 67.984)$; temp range 38.5 – $89.3^{\circ}C$, mercury as reference, Ambrose et al. 1975b)

$\log(P/kPa) = 6.22556 - 1628.007/(T/K - 66.119)$; temp range 74.9 – $190.8^{\circ}C$, water as reference, Ambrose et al. 1975b)

169.0 (calculated from different vapor eq., Ambrose et al. 1975)

160.5 (extrapolated-Antoine eq., Ambrose et al. 1979)

133.3 ($26.0^{\circ}C$, Verschuereen 1983)

160.5 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.21282 - 1618.669/(205.994 + t/^{\circ}\text{C})$; temp range 38.5–208°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

169.0 (Riddick et al. 1986)

$\log (P_L/\text{kPa}) = 5.56823 - 1197.54/(-115.829 + T/\text{K})$; temp range 348–452 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 7.4764 - 2455.4/(T/\text{K})$; temp range 273–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.20256 - 1611.255/(-67.979 + T/\text{K})$; temp range 409–481 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.48764 - 1782.204/(-52.863 + T/\text{K})$; temp range 311–376 K (Antoine eq.-IV, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.22745 - 1629.229/(-65.993 + T/\text{K})$; temp range 370–475 K (Antoine eq.-V, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 28.4711 - 3.4489 \times 10^3/(T/\text{K}) - 6.8363 \cdot \log (T/\text{K}) - 2.8173 \times 10^{-10} \cdot (T/\text{K}) + 9.5236 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 247–695 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.781, 1.494 (quoted exptl., calculated-bond contribution, Hine & Mookerjee 1975)

2.815 (Gaffney et al. 1987)

2.71* (gas stripping-GC, measured range 15–45°C, Betterton & Hoffmann 1988)

2.282* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -5.00 + 1977/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)

$\ln [K_H'/(M/\text{atm})] = -5.90 + 2207/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)

3.08* (EPICS-UV spectroscopy, measured range 5–25°C, Allen et al. 1998)

$\ln K_{AW} = -6759/(T/\text{K}) + 15.93$ (EPICS-UV, temp range 5–25°C, Allen et al. 1998)

1.94 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = 4.665 - 2276/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.48 (Leo et al. 1971; Hansch et al. 1972)

1.45 (shake flask-UV at pH 5.62, Umeyama et al. 1971)

1.43 (shake flask-UV, Holmes & Lough 1976)

1.45 ± 0.03 (shake flask at pH 7, Unger et al. 1978)

2.33 (HPLC-RT correlation, Veith et al. 1979)

1.56 (HPLC- k' correlation, Eadsforth 1986)

1.49 (shake flask, Eadsforth 1986)

1.44 (HPLC-RT correlation average, Ge et al. 1987)

1.54 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

1.48 (recommended, Sangster 1989, 1993)

1.72 (shake flask-UV, Kramer & Henze 1990)

1.48 (shake flask-UV spec., Alcron et al. 1993)

1.48 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: loss rate $k = 3.4 \times 10^{-4} \text{ min}^{-1}$ in outdoor Teflon chambers in dark (Grosjean 1985).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

$k < 2.0 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation by singlet oxygen in the aquatic systems at 25°C with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{OH}} = 1.3 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ determined by the long-path Fourier transform IR spectroscopic method with reference to that for C_2H_4 or C_2D_4 (Niki et al. 1978)

$k_{\text{OH}} = 7.6 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 0.74 \text{ d}$ (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{\text{OH}} = 7.8 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman 1982)

$k = (2.5 \pm 0.5) \text{ M}^{-1} \text{ s}^{-1}$ for 2–10 mM to react with ozone in water at pH 1.7 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{\text{NO}_3} = < 9.6 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (using relative rate technique to propene Carter et al. 1981; quoted, Atkinson 1991)

$k_{\text{NO}_3} = (2.55 \pm 0.08) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{NO}_3} = (1.13 \pm 0.25) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, compared to a previous measured value $k_{\text{NO}_3} < 5.2 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (relative rate technique, Atkinson et al. 1984)

$k_{\text{OH}} = .2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = 2.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ (reevaluated value, Atkinson et al. 1987)

$k_{\text{OH}}(\text{exptl}) = 1.30 \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 1.698 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (SAR, Atkinson 1987, 1990; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{NO}_3} = 2.54 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 1.29 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 11.40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $119.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976),

biodegradation rate constant $k = 0.065\text{--}0.074 \text{ h}^{-1}$ in 30 mg/L activated sludge after a lag time of 5–10 h (Urano & Kato 1986b).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9 \text{ d}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 0.74 \text{ d}$ based on rate constants for oxidation by OH radical in the atmosphere at 25°C (Mill 1982);

loss rate $k = (3.4 \pm 1.7) \times 10^{-4} \text{ min}^{-1}$ in outdoor Teflon chambers in the dark (Grosjean 1985);

calculated lifetimes of 11 h and 18 d for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.1.7.1
Reported aqueous solubilities of benzaldehyde at various temperatures

Stephenson 1993

shake flask-GC/TC

$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	8400
20.0	7200
30.0	7400
40.0	7900
50.0	8200
60.0	9300
70.0	10200
80.0	12400
90.0	14000

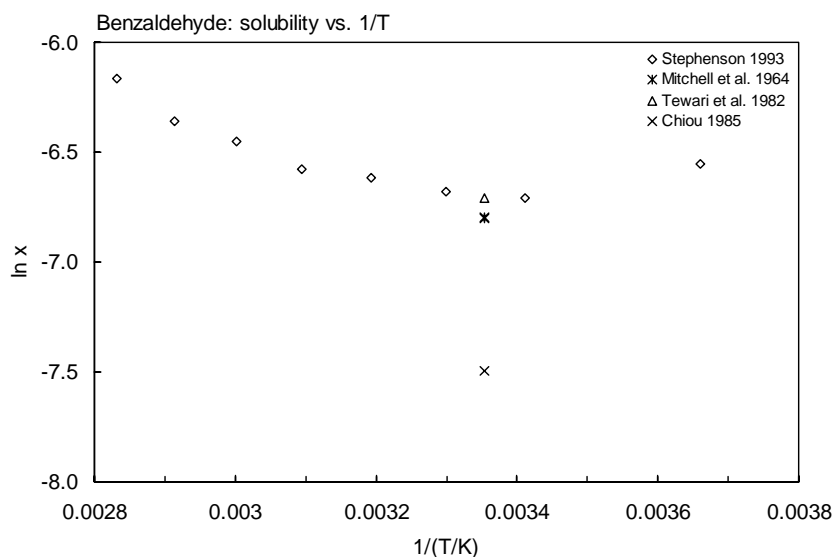


FIGURE 12.1.1.7.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for benzaldehyde.

TABLE 12.1.1.7.2

Reported vapor pressures of benzaldehyde at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947

Ambrose et al. 1975b

summary of literature data		comparative ebulliometry					
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
		mercury as reference		water as reference			
26.2	133.3	38.489	399	74.961	2837	25.0	169
50.1	666.6	41.273	473	77.570	3203	31.69	2000
62.0	1333	43.525	539	80.848	3723	76.85	3098
75.0	2666	45.584	608	85.231	4524	178.75	101325
90.1	5333	47.296	672	89.154	5352	213.35	225300
99.6	7999	48.838	722	93.610	6460	254.65	500000
112.5	13332	50.707	814	97.721	7644	421.65	4650000
131.7	26664	51.955	873	102.170	9124		
154.1	53329	56.352	1235	106.662	10854	bp/ $^{\circ}\text{C}$	178.75
179.0	101325	63.266	1592	111.251	12894		
		68.412	2057	115.947	15306	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
mp/ $^{\circ}\text{C}$	-26	75.098	2808	120.430	17945	at 25 $^{\circ}\text{C}$	50.3
		77.665	3150	126.350	21995	at bp	42.6
		80.998	3724	131.273	25910		
		83.392	4528	137.178	31339	density	
		89.251	5353	142.836	37379	T/K	$\rho/\text{kg m}^{-3}$
				148.806	44737	292.94	1044.85
				155.366	54140	298.09	1040.13
		Antoine eq.		161.067	63540	298.03	1040.22
		eq. 3	P/kPa	167.121	74923		

TABLE 12.1.1.7.2 (Continued)

Stull 1947		Ambrose et al. 1975					
summary of literature data		comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		A	6.20251	173.661	88998		
		B	1611.217	178.672	101131		
		C	-67.984	179.710	103800		
				185.556	119891		
				190.829	136055		
				Antoine eq.			
				eq. 3		P/kPa	
				A		6.22556	
				B		1628.007	
				C		-66.119	

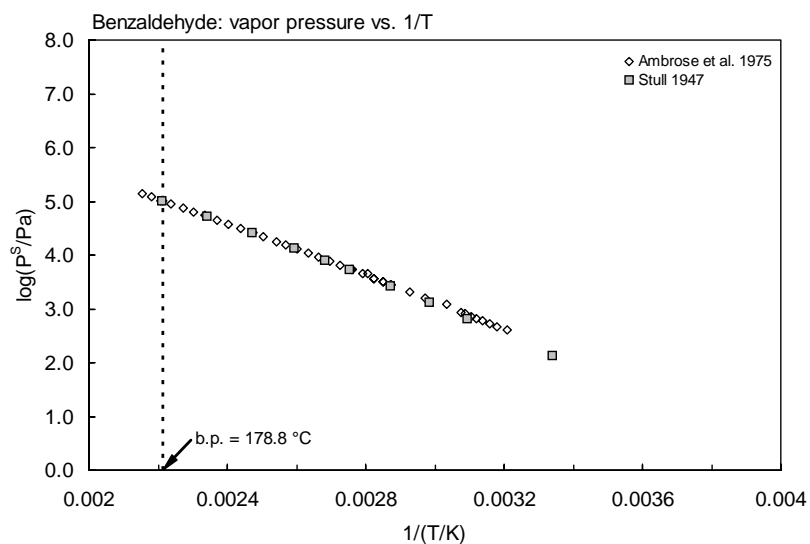


FIGURE 12.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for benzaldehyde.

TABLE 12.1.1.7.3

Reported Henry's law constants of benzaldehyde at various temperatures and temperature dependence equations

$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln [H/(\text{Pa m}^3/\text{mol})] &= A - B/(T/K) & (4) & \ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K) & (4a) \\ K_{AW} &= A - B\cdot(T/K) + C\cdot(T/K)^2 & (5) & & \end{aligned}$$

Zhou & Mopper 1990		Zhou & Mopper 1990		Betterton & Hoffmann 1988		Allen et al. 1998	
gas stripping-HPLC/UV		gas stripping-HPLC/UV		gas stripping-GC, spec.		EPICS-UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
	fresh water		sea water				
10	1.095	10	1.339	15	1.506	5	0.555
17	-	17	1.987	25	2.709	10	0.824
25	2.282	25	3.025	35	4.648	15	1.197
30	3.016	30	4.187	45	7.916	20	1.803
35	3.943	35	5.790			25	3.10
40	-	40	7.342				
45	6.413	45	9.296		$\Delta H/(\text{kJ mol}^{-1}) = -42.2$ at 25°C	eq. 1	K_{AW}
eq. 1a	$K_H'/(M/\text{atm})$	eq. 1a	$K_H'/(M/\text{atm})$			A	-6759
A	-5.00	A	-5.90			B	15.93
B	-1977	B	-2207				$\Delta H/(\text{kJ mol}^{-1}) = -56.2$ $\Delta S/(\text{J K}^{-1} \text{mol}^{-1}) = 132.4$

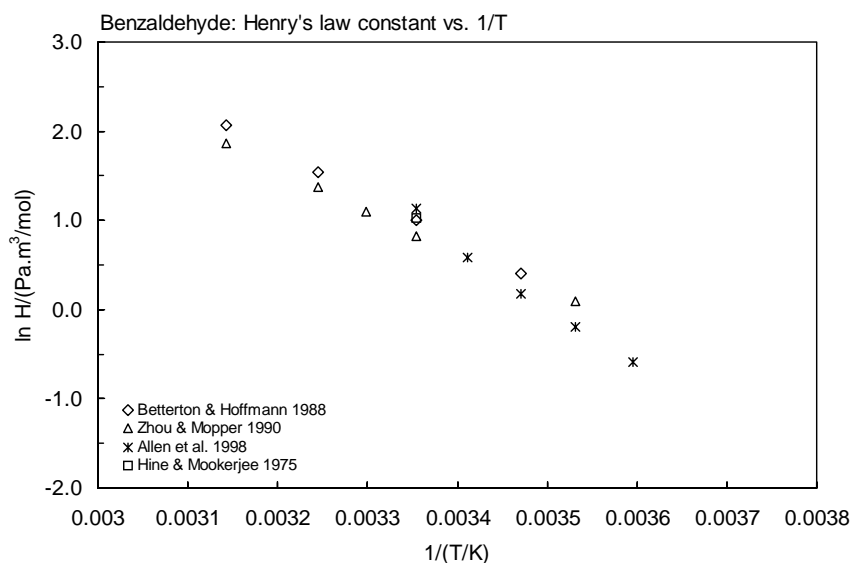


FIGURE 12.1.1.7.3 Logarithm of Henry's law constant versus reciprocal temperature for benzaldehyde.

12.1.2 KETONES

12.1.2.1 Acetone



Common Name: Acetone

Synonym: 2-propanone, dimethylketone, DMK

Chemical Name: acetone, 2-propanone

CAS Registry No: 67-64-1

Molecular Formula: C_3H_6O , CH_3COCH_3

Molecular Weight: 58.079

Melting Point ($^{\circ}C$):

−94.7 (Lide 2003)

Boiling Point ($^{\circ}C$):

56.05 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7899 (Weast 1982–83)

0.7908 (Dean 1985)

Molar Volume (cm^3/mol):

73.5 ($20^{\circ}C$, calculated-density)

74.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

5.690 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

miscible ($20^{\circ}C$, Palit 1947)

miscible (Dean 1985; Yaws et al. 1990)

miscible (Riddick et al. 1986; Howard 1990)

217700, 453000 (pseudo-solubilities, Staples 2000)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29610* (interpolated-regression of tabulated data, temp range -59.4 to $56.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.19038 - 1233.4/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

30490 (Perry 1950)

51854* ($37.68^{\circ}C$, temp range 37.68 – $56.02^{\circ}C$, Brown & Smith 1957)

30800 (Buttery et al. 1969)

30810 (Hoy 1970)

29923* ($24.330^{\circ}C$, temp range -12.949 to $55.285^{\circ}C$, Boublik & Aim 1972; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 10577.7/(T/K)] + 9.143231$; temp range -20 to $96^{\circ}C$ (Antoine eq., Weast 1972–73)

30780, 30800 (calculated-Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.15853 - 1231.232/(231.766 + t/^{\circ}C)$; temp range 37.6 – $56.02^{\circ}C$ (Antoine eq. from reported exptl. data of Brown & Smith 1957, Boublik et al. 1973)

$\log(P/mmHg) = 7.11714 - 1210.595/(229.664 + t/^{\circ}C)$; temp range -12.95 to $55.3^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

30810* (ebulliometry, fitted to Antoine eq., measured range 259 – $350.9 K$, Ambrose et al. 1974)

$\log(P/kPa) = 6.25632 - 1217.904/(T/K - 42.692)$; temp range 311.7 – $350.9 K$, or for pressure range 53 – $202 kPa$ (Antoine eq., ebulliometry, Ambrose et al. 1975a)

$\log(P/kPa) = 6.25478 - 1216.689/(T/K - 42.875)$; temp range 259.17 – $350.9 K$, or for pressure below $225 kPa$ (Antoine eq., ebulliometry, Ambrose et al. 1974)

30870, 31520 (quoted exptl., calculated-Antoine eq., Boublik et al. 1984)

- $\log (P/\text{kPa}) = 6.24039 - 1209.746/(229.574 + t/^{\circ}\text{C})$; temp range -12.95 to 55.3°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.26017 - 1214.208/(230.002 + t/^{\circ}\text{C})$; temp range -13.98 to 77.72°C (Antoine eq. from reported exptl. data of Ambrose et al. 1974, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.28185 - 1230.342/(231.665 + t/^{\circ}\text{C})$; temp range 37.6 – 56.02°C (Antoine eq. from reported exptl. data of Brown & Smith 1957, Boublik et al. 1984)
 30780 (calculated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.11714 - 1210.595/(229.664 + t/^{\circ}\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
 24227, 30806 (20, 25°C , Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.25478 - 1216.589/(230.275 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 30730 (interpolated-Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24204 - 1210.6/(-43.49 + T/\text{K})$; temp range 261–329 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.75622 - 1566.69/(0.269 + T/\text{K})$; temp range 329–488 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 3.6452 - 469.5/(-108.21 + T/\text{K})$; temp range 178–243 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19735 - 1190.382/(-45.373 + T/\text{K})$; temp range 203–269 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.26483 - 1221.852/(-42.388 + T/\text{K})$; temp range 257–334 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24554 - 1211.515/(-43.471 + T/\text{K})$; temp range 323–379 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.69966 - 1542.465/(0.447 + T/\text{K})$; temp range 374–464 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 28.5884 - 2.469 \times 10^3/(T/\text{K}) - 7.351 \cdot \log (T/\text{K}) + 2.8025 \times 10^{-10} \cdot (T/\text{K}) + 2.7361 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 178–508 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 3.34 (partial pressure, Butler & Ramchandani 1935)
 3.96 (shake flask, partial vapor pressure-GC, Burnett 1963)
 3.25 (28°C , concn. ratio-GC, Nelson & Hoff 1968)
 3.97 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 4.02, 3.93, 2.91 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 4.05 (headspace-GC, Vitenberg et al. 1975)
 4.10 (calculated-activity coeff and vapor pressure, γ -P, Rathbun & Tai 1982)
 0.908, 3.93 (0, 25°C , headspace-GC, Snider & Dawson 1985)
 3.38 (review, Gaffney et al. 1987)
 2.928* (gas-stripping-HPLC-UV, measured range 10 – 45°C , Zhou & Mopper 1990)
 $\ln [K_H'/(M/\text{atm})] = -5.00 + 1977/(T/\text{K})$; temp range 10 – 45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
 $\ln [K_H'/(M/\text{atm})] = -3.60 + 1518/(T/\text{K})$; temp range 25 – 45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 11), Zhou & Mopper 1990)
 3.07* (gas stripping-GC, measured range -14.9 to 44.9°C , Betterton 1991)
 4.33 (computed, Yaws et al. 1991)
 0.722, 1.26, 2.045, 5.31, 7.514 (0.51, 9.0, 16.11, 31, 38.51°C , headspace-GC, de-ionized water, Benkelberg et al. 1995)
 3.735* (headspace-GC, rain water, measured range -30 to 39.51°C , Benkelberg et al. 1995)
 0.762, 2.19, 6.64, 10.30 (0, 14.51, 30, 39.51°C , headspace-GC, artificial seawater, Benkelberg et al. 1995)
 $\ln (k_H/\text{atm}) = (18.4 \pm 0.3) - (5386 \pm 100)/(T/\text{K})$, temp range 10 – 40°C (headspace-GC measurements, Benkelberg et al. 1995)
 2.56 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 1996)
 9.92 (EPICS-GC, Ayuttaya et al. 2001)
 2.58 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 3.742 - 1965/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{ow} :

-0.24	(shake flask-CR, Collander 1951)
-0.24	(shake flask at pH 7, Unger et al. 1978)
-0.48	(shake flask-GC, Tani et al. 1986)
-0.24	(recommended, Sangster 1989, 1993)
-0.31	(CPC centrifugal partition chromatography, Gluck & Martin 1990)
-0.37	(calculated-UNIFAC activity coeff., Dallos et al. 1993)
-0.24	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

2.31	(head-space GC, Abraham et al. 2001)
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Bioconcentration Factor, log BCF:

-0.187	(calculated, Staples 2000)
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Sorption Partition Coefficient, log K_{OC} :

-0.586	(calculated- K_{ow} , Kollig 1993)
-0.523	(quoted calculated value, Staples 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 20$ h was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: rate constant $k = 1.4 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carlier et al. 1986); calculated lifetime $\tau \sim 60$ d in air (Atkinson 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius expression see reference:

photooxidation $t_{1/2} = 11.3\text{--}453$ yr, based on measured data for the reaction with hydroxyl radical in aqueous solution (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} > 9.9$ d for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)

$k_{OH} = (0.23 \pm 0.03) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (flash photolysis-resonance fluorescence, Zetzsch 1982; quoted, Atkinson 1985)

$k_{OH} = (0.62 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (relative rate technique to *n*-hexane, Chiorboli et al. 1983; quoted, Atkinson 1985)

$k = 0.032 \pm 0.006 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 2.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 279\text{--}2790$ h, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)

$k_{OH} = 2.16 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k = 1.80 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the aqueous-phase reaction with hydroxyl radical in solution (Wallington & Kurylo 1987)

$k_{OH} = 2.16 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 1.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH}^* = 2.26 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 0.18 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: biodegradation rate constants, $k = 0.016\text{--}0.020 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 20–25 h (Urano & Kato 1986b);

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168$ h, based on unacclimated aqueous screening test data (Bridie et al. 1979; Dore et al. 1975; selected, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$k(\text{exptl}) = 0.0440 \text{ h}^{-1}$ compared to predicted rate constants by group contribution method: $k = 0.0433 \text{ h}^{-1}$ (nonlinear) and $k = 0.043 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} > 9.9 \text{ d}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 279\text{--}2790 \text{ h}$, based on measured data for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

calculated lifetimes $\tau = 53 \text{ d}$ and $\tau > 11 \text{ yr}$ for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000);

photooxidation and photolysis $t_{1/2} = 36 \text{ h}$ (Staples 2000).

Surface water: photooxidation $t_{1/2} = 11.3\text{--}453 \text{ yr}$, based on measured data for the reaction with hydroxyl radicals in aqueous solution (Dorfman & Adams 1973; quoted, Howard et al. 1991);

$t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

aerobic biodegradation $t_{1/2} = 96\text{--}168 \text{ h}$ (Staples 2000).

Ground water: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: anaerobic biodegradation $t_{1/2} = 384 \text{ h}$ or 16 d (Staples 2000).

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

aerobic biodegradation $t_{1/2} = 96\text{--}168 \text{ h}$ (Staples 2000).

Biota:

TABLE 12.1.2.1.1

Reported vapor pressures of acetone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Stull 1947		Brown & Smith 1957		Boublik & Aim 1972			
summary of literature data		Austr. J. Chem. 10, 423-		ref. in Boublik et al. 1984*			
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
-59.4	133.3	37.68	51854	-12.949	4524	36.649	49704
-40.5	666.6	41.58	60127	-5.424	6967	42.094	61295
-31.1	1333	44.96	68271	-0.103	9306	48.344	77125
-20.8	2666	45.0	68367	4.882	12046	55.285	98572
-9.40	5333	47.01	73603	8.666	14549	bp/ $^{\circ}\text{C}$	56.102
-2.0	7999	49.31	79969	13.019	17921	Antoine eq. eq. 2	
7.7	13332	51.91	87727	16.831	21314		P/kPa
22.7	26664	56.02	101199	20.939	25780		6.24039
39.5	53329			24.330	29923		1209.746
56.5	101325			28.351	35493		229.574
				32.138	41470	C	
mp/ $^{\circ}\text{C}$	-94.6						

*ref. Collection Czech. Chem. Commun 37, 3513 (1972)

TABLE 12.1.2.1.1 (Continued)

2.

Ambrose et al. 1974

comparative ebulliometry

t/°C	P/Pa	t/°C	P/Pa
		cont'd	
-13.975	4257	55.876	100666
-11.019	5076	56.646	103344
-8.106	6005	60.963	119433
-4.982	7186	64.859	135602
-1.388	8691	69.512	157101
0.288	9497	73.943	180024
1.972	10376	77.724	201571
2.007	10391	25.0	30806
5.493	12417		
5.511	12432	eq. 3	P/kPa
9.077	14840	A	6.25478
9.093	14851	B	1216.689
12.473	17480	C	-42.875
16.928	21525		
20.717	25544		
25.045	30867	Ambrose et al 1975a	
29.275	36912		
33.720	44267	bp/°C	56.067
28.601	53675		
42.834	63079	eq. 3	P/kPa
47.320	74449	A	6.25632
52.170	88536	B	1217.904
		C	-42.692
		equation for vapor pressures below 200 kPa	
		$\Delta H_v / (\text{kJ mol}^{-1}) =$	
		at 25°C	31.3
		at bp	29.6

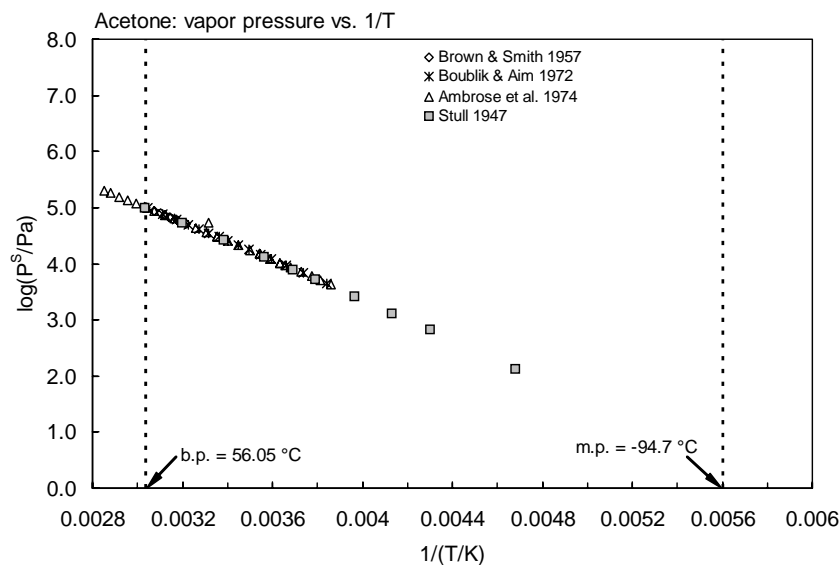


FIGURE 12.1.2.1.1 Logarithm of vapor pressure versus reciprocal temperature for acetone.

TABLE 12.1.2.1.2
Reported Henry's law constants of acetone at various temperatures and temperature dependence equations

$$\ln K_{AW} = A - B/(T/K)$$
$$\ln (1/K_{AW}) = A - B/(T/K)$$
$$\ln (k_H/\text{atm}) = A - B/(T/K)$$
$$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$$
$$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$$

$$\log K_{AW} = A - B/(T/K)$$
$$\log (1/K_{AW}) = A - B/(T/K)$$
$$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$$

$$(1)$$
$$(2)$$
$$(3)$$
$$(4)$$
$$(5)$$

$$(1a)$$
$$(2a)$$
$$(4a)$$

1.

Snider & Dawson 1985		Zhou & Mopper 1990				Betterton 1991	
gas stripping-GC/FID		gas stripping-HPLC/UV		gas stripping-HPLC/UV		gas stripping-GC/FID	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)
		fresh water		sea water			
0	0.908	10	1.421	10	1.735	14.9	2.303
25	3.935	17	-	17	2.356	25	3.070
		25	2.846	25	3.311	25	3.269
		30	3.658	30	4.037	25	3.897
enthalpy of transfer		35	4.585	35	4.825	25	3.753
ΔH =	37.24 kJ/mol	40	-	40	5.537	25	3.958
		45	6.178	45	6.846	35.1	7.794
						44.9	11.92
		eq. 1a	K _H '/(M/atm)	eq. 1a	k _H '/(M/atm)		
		A	-5.00	A	-3.60		
		B	-1977	B	-1518		

TABLE 12.1.2.1.2 (Continued)

2.

Benkelberg et al. 1995

equilibrium vapor phase concentration-headspace GC

t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
deionized water		rain water	
0.51	0.7222	−28.0	0.742
9.0	1.260	25.0	3.735
16.61	2.0445	39.51	8.328
31.0	5.313		
38.51	7.514	artificial sea water	
		0	0.757
for deionized and rain water:		14.51	2.189
eq. 3	k _H /atm	30.0	6.639
A	18.4 ± 0.3	39.51	10.305
B	5286 ± 100		

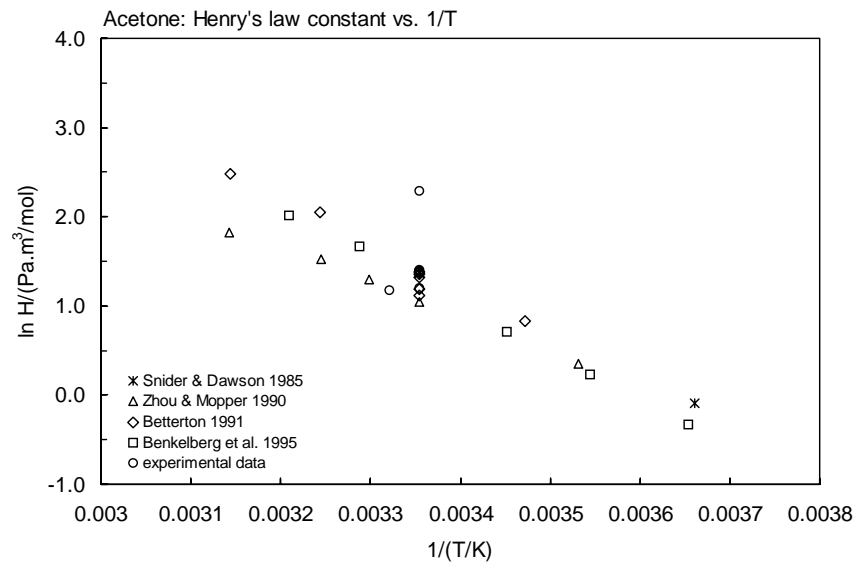


FIGURE 12.1.2.1.2 Logarithm of Henry's law constant versus reciprocal temperature for acetone.

12.1.2.2 2-Butanone (Methyl ethyl ketone)



Common Name: Methyl ethyl ketone

Synonym: 2-butanone, butan-2-one, MEK

Chemical Name: 2-butanone, methyl ethyl ketone

CAS Registry No: 78-93-3

Molecular Formula: C_4H_8O , $CH_3CH_2COCH_3$

Molecular Weight: 72.106

Melting Point ($^{\circ}C$):

−86.64 (Lide 2003)

Boiling Point ($^{\circ}C$):

79.59 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8054 (Weast 1982–83)

0.7997 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

89.9 (calculated-density, Rohrschneider 1973)

96.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

14.7 (pK_a , Riddick et al. 1986)

−7.2 (pK_{BH}^+ , Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

8.439 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

240000 ($20^{\circ}C$, synthetic method, Jones 1929; quoted, Palit 1947; Dean 1985; Riddick et al. 1986)

255700* (shake flask-volumetric method, measured range 20 – $30^{\circ}C$ Ginnings et al. 1940)

343550 (shake flask-volumetric, Ginnings et al. 1940)

228020 (estimated, McGowan 1954)

12420 ($20^{\circ}C$, Amidon et al. 1975)

136280 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

353000 ($20^{\circ}C$, Verschueren 1983)

249000 (selected, Yaws et al. 1990)

276000*, 235000 ($19.3^{\circ}C$, $29.7^{\circ}C$, shake flask-GC, measured range 0 – $70.2^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

12954* (interpolated-regression of tabulated data, temp range -48.3 to $79.6^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.22200 - 1343.6/(230 + t/^{\circ}C)$, (Antoine eq., Dreisbach & Martin 1949)

16500* ($31.84^{\circ}C$, ebulliometry, measured range 31.84 – $79.5^{\circ}C$, Dreisbach & Shrader 1949)

25158* ($41.46^{\circ}C$, flow calorimetry, measured range 41.46 – $79.5^{\circ}C$, Nickerson et al. 1961)

26568* ($42.778^{\circ}C$, ebulliometry, measured range 42.778 – $88.444^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.06376 - 1261.455/(221.982 + t/^{\circ}C)$; temp range 42.778 – $88.444^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 19.48322 - 2328.0/(T/K) - 3.92657 \cdot \log(T/K)$; temp range 42.778 – $88.444^{\circ}C$ (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = [-0.2185 \times 8149.5/(T/K)] + 7.959295$; temp range -48.3 to $79.6^{\circ}C$ (Antoine eq., Weast 1972–73)

- 12079* (ebulliometry, Ambrose et al. 1975a; quoted, Riddick et al. 1986; Howard 1990)
 12000, 12060, 12640 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.02273 - 1167.861/(211.199 + t/^{\circ}\text{C})$; temp range 41.46–97.42°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.18397 - 1258.948/(221.725 + t/^{\circ}\text{C})$; temp range 42.78–86.44°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.18838 - 1261.297/(222.964 + t/^{\circ}\text{C})$; temp range 42.79–88.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 12020 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.06356 - 1261.34/(221.97 + t/^{\circ}\text{C})$; temp range 43–88°C (Antoine eq., Dean 1985, 1992)
 12700 (Howard et al. 1986; quoted, Banerjee et al. 1990)
 12120 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.24715 - 1294.53/(-47.442 + T/\text{K})$; temp range 294–352 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.18479 - 1259.519/(-51.359 + T/\text{K})$; temp range 315–363 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.22518 - 1286.794/(-47.766 + T/\text{K})$; temp range 353–403 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 5425 (calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 47.706 - 3.0965 \times 10^3/(T/\text{K}) - 15.184 \cdot \log(T/\text{K}) + 7.4846 \times 10^{-3} \cdot (T/\text{K}) - 1.7084 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 186–536 K (vapor pressure eq., Yaws 1994)
 12071* (static method-manometry, measured range 0–50°C, Garriga et al. 1996)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 4.710 (shake flask, partial vapor pressure-GC, Buttery et al. 1969)
 4.723 (quoted, exptl., Hine & Mookerjee 1975)
 5.549, 4.408 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 3.87 (headspace-GC, Vitenberg et al. 1975)
 6.191, 4.215 (calculated- γ -P, calculated-MW, Rathbun & Tai 1982)
 0.987, 5.76 (0, 25°C, gas stripping-GC, Snider & Dawson 1985)
 13.17* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln[H/(\text{atm} \cdot \text{m}^3/\text{mol})] = -26.32 - 5214/(T/\text{K})$, temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)
 5.210 (gas stripping-HPLC/UV, Zhou & Mopper 1990)
 5.117* (gas-stripping-HPLC-UV, measured range 10–45°C, Zhou & Mopper 1990)
 $\ln[K_H'/(M/\text{atm})] = -6.03 + 2184/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, freshwater, Zhou & Mopper 1990)
 $\ln[K_H'/(M/\text{atm})] = -5.97 + 2138/(T/\text{K})$, temp range 10–45°C (gas stripping-HPLC measurements, seawater (salinity 35 ± 1 l), Zhou & Mopper 1990)
 18.28* (45°C, equilibrium headspace-GC, measured range 45–80°C, Ettre et al. 1993)
 $\log(1/K_{AW}) = -3.7973482 + 1889.5294/(T/\text{K})$, temp range 45–80°C (equilibrium headspace-GC measurements, Ettre et al. 1993)
 3.85 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 3.95 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 4.764 - 2213/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)
 5.04 – 3.54 (27°C, equilibrium headspace-GC, solute concn 10.01–85.10 mg/L, measured range 300–315 K, Cheng et al. 2003)
 5.04* (27°C, equilibrium headspace-GC, measured range 27–42°C, Cheng et al. 2003)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.26 (shake flask-CR, Collander 1957)
 0.28 (shake flask-UV, Fujita et al. 1964, Hansch & Leo 1979)
 0.32 ± 0.01 (shake flask-UV, calculated, Iwasa et al. 1965)
 0.29 (shake flask-UV, GC, Hansch & Anderson 1967; Hansch et al. 1968; Leo et al. 1969, 1971)
 0.28 ± 0.02 (shake flask at pH 7, Unger et al. 1978)

0.69	(generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
0.26	(shake flask-GC, Tanii et al. 1986)
0.62	(calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
0.29	(recommended, Sangster 1989, 1993)
0.29	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.77	(head-space GC, Abraham et al. 2001)
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Bioconcentration Factor, $\log BCF$:

0.00	(estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
------	--

Sorption Partition Coefficient, $\log K_{OC}$:

1.53	(soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)
1.47 ± 0.55 , 1.53 ± 0.88 ; 1.50	(Captina silt loam, McLaurin sandy loam; weighted mean, batch equilibrium-sorption isotherm, Walton et al. 1992)
0.070	(predicted- K_{OW} , Walton et al. 1992)
-0.03	(calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on lab. data for evaporation relative to the reaeration rate of 0.27 (Mackay et al. 1982; Rathbun & Tai 1982; quoted, Howard 1990) and typical reaeration rates of rivers and lakes (Mill et al. 1982; quoted, Howard 1990),

$t_{1/2} = 3$ d for evaporation from a river and $t_{1/2} = 12$ d from lake (Howard 1990).

Photolysis: rate constant $k = 1.4 \times 10^{-5} \text{ s}^{-1}$ in the atmosphere (Carrier et al. 1986); calculated lifetime $\tau \sim 4$ d in air (Atkinson 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

photooxidation $t_{1/2} = 48.8 - 81.4$ yr, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 2.4 - 24$ h in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976)

$k_{OH} = (0.20 \pm 0.06) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

$k < 2.0 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation with singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 00$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 1.9 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 2.9$ d (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{OH} = (0.95 \pm 0.09) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at (295 ± 2) K in air (relative rate technique to ethene Cox et al. 1981; quoted, Atkinson 1985)

$k_{OH} = (1.20 \pm 0.20) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K in air (flash photolysis-resonance fluorescence, Zetzsch 1982; quoted, Atkinson 1985)

$k = (0.12 \pm 0.02) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 20–300 mM *t*-BuOH as scavenger at pH 2 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983)

$k_{OH}(\text{calc}) = 1.38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 0.97 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 24°C with an atmospheric lifetime $\tau = 12$ d (Edney et al. 1986)

$k_{OH} = 1.15 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k(\text{soln}) = 1.50 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the aqueous-phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{OH}^* = 1.15 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

photooxidation $t_{1/2} = 64.2 - 642$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Howard et al. 1991)

$k_{OH}(\text{calc}) = 1.65 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: first-order hydrolysis $t_{1/2} > 0$ yr, based on nonreactive hydrolysis from pH 5 to 9 at 15°C (Kollig et al. 1987; selected, Howard et al. 1991).

Biodegradation:

$k = 0.021 - 0.025 \text{ h}^{-1}$ in 30 mg/L activated sludge after a time lag of 5 h (Urano & Kato 1986b)

$t_{1/2}(\text{aq. aerobic}) = 24 - 168 \text{ h}$, based on unacclimated grab sample of aerobic freshwater (Dojlido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96 - 672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4 - 24 \text{ h}$ in air for the gas-phase reaction with hydroxyl radical, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 9.8 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976)

$t_{1/2} = 2.3 \text{ d}$ for the atmospheric reaction with photochemically produced hydroxyl radical (Cox et al. 1981; quoted, Howard 1990);

photooxidation $t_{1/2} = 64.2 - 642 \text{ h}$, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);

calculated atmospheric lifetime $\tau = 12 \text{ d}$ due to reaction with OH radical (Edney et al. 1986) atmospheric transformation lifetime $\tau < 1 \text{ d}$ (estimated, Kelly et al. 1994);

calculated lifetime $\tau = 10 \text{ d}$ for reaction with OH radical (Atkinson 2000).

Surface water: photooxidation $t_{1/2} = 48.8 - 81.4 \text{ yr}$, based on measured rate data for the reaction with hydroxyl radical in aqueous solution (Anbar & Neta 1967; quoted, Howard et al. 1991); $t_{1/2} = 24 - 168 \text{ h}$, based on unacclimated grab sample of aerobic freshwater (Dojlido 1979; selected, Howard et al. 1991) and aerobic aqueous screening test data (Takemoto et al. 1981; selected, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995).

Ground water: $t_{1/2} = 48 - 336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: calculated $t_{1/2} = 4.9 \text{ d}$ from first-order kinetic of degradation under both sterile and nonsterile conditions (Anderson et al. 1991);

$t_{1/2} = 24 - 168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.2.2.1

Reported aqueous solubilities of 2-butanone (methyl ethyl ketone) at various temperatures

Ginnings et al. 1940		Stephenson 1992	
volumetric method		shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
20	273300	0	367000
25	255700	9.6	310000
30	240700	19.3	276000
		29.7	245000
bp/ $^{\circ}\text{C}$	80.7–80.8	39.6	220000
d ²⁵	0.8007	49.7	206000
		60.6	180000
		70.2	182000

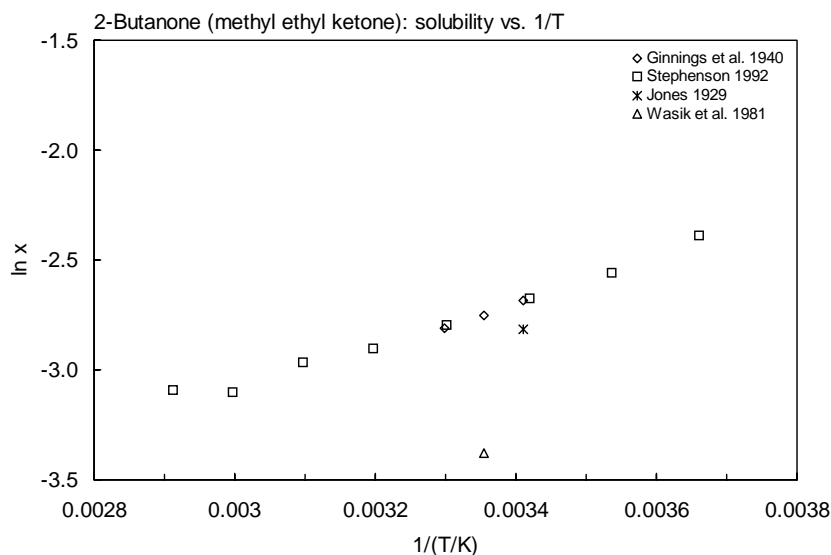


FIGURE 12.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.2

Reported vapor pressures of 2-butanone (methyl ethyl ketone) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

1.

Stull 1947		Dreisbach & Shrader 1949		Nickerson et al. 1961		Collerson et al. 1965	
summary of literature data		ebulliometry		flow calorimetry		ebulliometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-48.3	133.3	31.84	16500	41.46	25158	42.778	26568
-28.0	666.6	54.29	42066	65.54	63368	48.148	33024
-17.7	1333	67.36	67661	79.39	101098	53.026	39963
-6.50	2666	79.5	101325	89.43	137282	57.08	46591
6	5333			97.42	173212	60.821	53469
14	7999					64.005	59954
25	13332			eq. 4	P/mm Hg	67.009	66625
41.6	26664			A	21.78963	69.734	73184
60	53329			B	2441.9	72.343	79933
79.6	101325			C	4.70504	74.839	86849
						76.95	93063
mp/ $^{\circ}\text{C}$	-85.9					79.221	100135
						81.268	106887
						83.161	113428
						85.013	120126
						86.715	126547
						88.44	133353
						mp/ $^{\circ}\text{C}$	-86.69
						bp/ $^{\circ}\text{C}$	79.589

TABLE 12.1.2.2.2 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Nickerson et al. 1961		Collerson et al. 1965	
summary of literature data		ebulliometry		flow calorimetry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						Antoine eq.	
						eq. 2	P/mmHg
						A	7.06376
						B	1261.455
						C	221.982
						Kirchhoff eq.	
						eq. 4	P/mmHg
						A	19.48322
						B	2328
						C	3.92657
						$\Delta H_v/(\text{kJ mol}^{-1}) = 31.67$	

2.

Ambrose et al. 1975(a)		Garriga et al. 1996	
comparative ebulliometry		static method-manometry	
t/°C	P/Pa	t/°C	P/Pa
25	12079	5	4277
42.778	26568	10	5644
48.137	33023	15	7334
53.016	39963	20	9435
57.07	46591	25	12071
60.812	53468	30	15281
63.996	59953	35	19110
67.001	66625	40	23682
69.726	73184	45	29132
72.335	79933	50	35540
74.832	86848		
76.944	93063	Antoine eq.	
79.215	100136	eq. 3a	P/kPa
81.262	106887	A	14.133009
83.156	113427	B	2843.871
85.009	120125	C	−53.875
86.711	126545		
88.444	133352		
bp/°C	79.583		
eq. 2	P/kPa		
A	6.18444		
B	1259.223		
C	−51.392		
ΔH _v /(kJ mol ^{−1}) =			
at 25°C	34.7		
at bp	31.8		

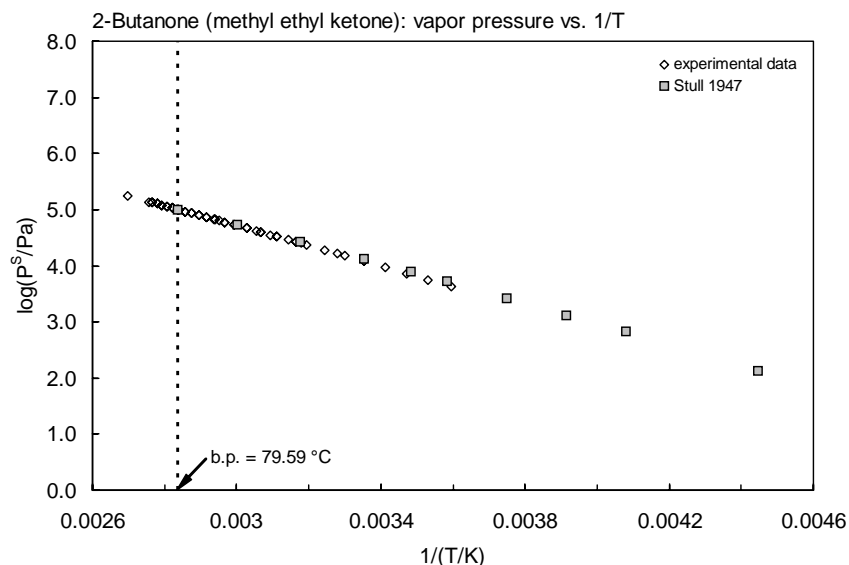


FIGURE 12.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 2-butanone.

TABLE 12.1.2.2.3

Reported Henry's law constants of 2-butanone (methyl ethyl ketone) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$	(1)	$\log K_{AW} = A - B/(T/K)$	(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$	(2)	$\log (1/K_{AW}) = A - B/(T/K)$	(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$	(3)		
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$	(4)	$\ln [H/(\text{atm} \cdot \text{m}^3/\text{mol})] = A - B/(T/K)$	(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$	(5)		

Snider & Dawson 1985		Ashworth et al. 1988		Zhou & Mopper 1990			
gas stripping-GC		EPICS-GC		gas stripping-HPLC/UV		gas stripping-HPLC/UV	
t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
0	0.9873	10	28.37	10	2.068	10	2.702
25	5.765	15	39.52	17	-	17	3.943
		20	19.25	25	5.117	25	6.666
enthalpy of transfer:		25	13.17	30	7.186	30	8.735
$\Delta H/(\text{kJ mol}^{-1}) = 46.024$		30	11.15	35	9.296	35	10.78
				40	-	40	14.07
		eq. 4a	H/(atm m ³ /mol)	45	14.27	45	18.09
		A	-26.32	eq. 1a	K _H '/(M/atm)	eq. 1a	K _H '/(M/atm)
		B	-5214	A	-6.03	A	-5.97
				B	-2184	B	-2138

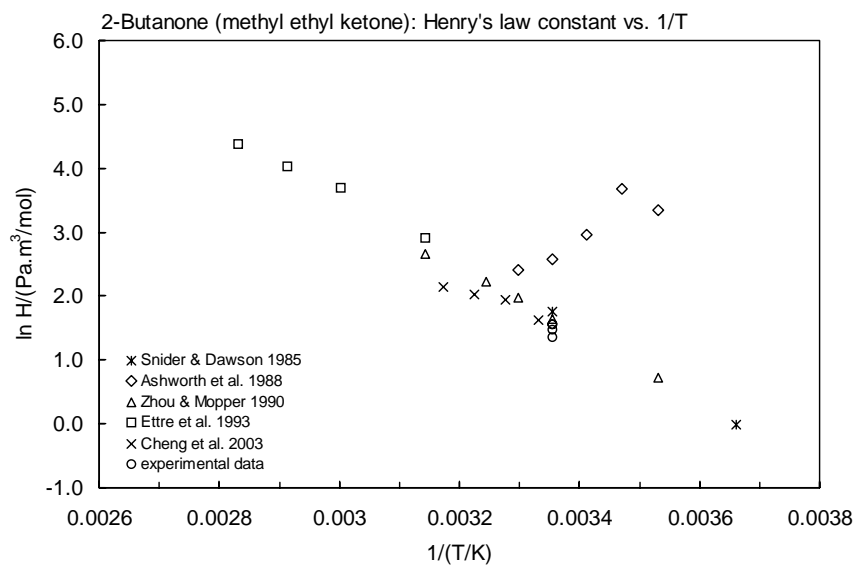
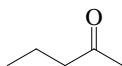


FIGURE 12.1.2.2.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-butanone.

12.1.2.3 2-Pentanone



Common Name: 2-Pentanone

Synonym: 2-pentanone, methyl propyl ketone, methyl *n*-propyl ketone, ethylacetone

Chemical Name: 2-pentanone, methyl propyl ketone

CAS Registry No: 107-87-9

Molecular Formula: C₅H₁₀O, CH₃CH₂CH₂COCH₃

Molecular Weight: 86.132

Melting Point (°C):

−77.80 (Stull 1947; Weast 1982–83; Dean 1985; Howard 1990)

−76.8 (Lide 2003)

Boiling Point (°C):

102.0 (Weast 1982–83; Verschueren 1983)

101.7 (Dean 1985; Howard 1990)

102.26 (Lide 2003)

Density (g/cm³ at 20°C):

0.8089 (Weast 1982–83)

0.8064, 0.8015 (20°C, 25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

118.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

2.541 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} J/mol K:

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

54268* (30°C, shake flask-interferometer, measured range 10–50°C, Gross et al. 1939)

30150 (30°C, Gross et al. 1939)

55100 (shake flask-volumetric, Ginnings et al. 1940)

59500 (20°C, shake flask-volumetric, Ginnings et al. 1940)

64010 (shake flask-interferometer, Donahue & Bartell 1952)

54350 (McGowan 1954; Deno & Berkheimer 1960)

43000 (Verschueren 1977, 1983)

59500 (20°C, Riddick et al. 1986)

55400 (selected, Yaws et al. 1990)

59000* (19.7°C, shake flask-GC, measured range 0–90.5°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2088* (interpolated-regression of tabulated data, temp range −12.7 to 102.7°C, Stull 1947)

2666 (28.5°C, Stull 1947)

20440* (56.649°C, ebulliometry, measured range 56.5–111.655°C, Collerson et al. 1965)

log (P/mmHg) = 7.01753 − 1311.145/(214.693 + t/°C); temp range 56.5–111.65°C (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

log (P/mmHg) = 21.71880 − 2694.12/(T/K) − 4.63307·log (T/K); temp range 56.5–111.65°C (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)

log (P/mmHg) = 6.13916 − 1379.06/(221.41 + t/°C); temp range −5 to 100°C (data fitted to Antoine eq., static method-Ramsey-Young apparatus measurements, Meyer & Wagner 1966)

log (P/mmHg) = [−0.2185 × 11240.6/(T/K)] + 9.432089; temp range −12–103.3°C (Antoine eq., Weast 1972–73)

4720* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)

2133 (quoted, Verschueren 1983)

- 1621 (quoted, Mackay & Yuen 1983)
 4648 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.14908 - 1311.372/(214.222 + t/^{\circ}\text{C})$, temp range 61.72–121.4°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = 7.02193 - 1313.85/(215.01 + t/^{\circ}\text{C})$, temp range 56–111°C (Antoine eq., Dean 1985, 1992)
 4702 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.14243 - 1311.145/(-58.457 + T/\text{K})$, temp range 329–386 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.1404 - 1310.269/(-58.514 + T/\text{K})$, temp range 336–422 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.47975 - 1569.596/(-24.035 + T/\text{K})$, temp range 416–501 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 18.3056 - 2.3477 \times 10^3/(T/\text{K}) - 3.6667 \cdot \log(T/\text{K}) + 7.1502 \times 10^{-4} \cdot (T/\text{K}) + 1.0912 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 196–561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 10.91 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
 6.44 (partial vapor pressure-GC, Buttery et al. 1969)
 6.52 (quoted, exptl., Hine & Mookerjee 1975)
 7.66, 6.52 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 3.83 (calculated- γ -P, Rathbun & Tai 1982)
 5.876 (gas-stripping, Hawthorne 1984)
 10.13 (modified gas-stripping, Hawthorne et al. 1985)
 8.47, 6.83 (gas stripping-GC, calculated-P/C, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.91 \pm 0.03 (shake flask-UV at pH 7, Unger et al. 1978)
 0.91 (Hansch & Leo 1985)
 0.78 (shake flask-GC, Tanii et al. 1986)
 0.87 (calculated- V_1 and solvatochromic parameters, Kamlet et al. 1988)
 0.95 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.84 (recommended, Sangster 1989; 1993)
 0.91 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 3.19 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.477 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.869 (soil, estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} = 15.5$ h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and $t_{1/2} = 14.5$ h in a wind-wave tank with a 6m/s wind speed (Howard 1990).
 Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976)
 $k_{OH} = (4.64 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(299 \pm 2) \text{ K}$ (relative rate technique to cyclohexane Atkinson et al. 1982; quoted, Atkinson 1985)
 $k \sim 0.02 \text{ M}^{-1} \cdot \text{s}^{-1}$ for the reaction with ozone in water at pH 2 and 20–23°C (Hoigné & Bader 1983)

$k_{\text{OH}}(\text{calc}) = 4.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 4.64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}} = 4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k(\text{soln}) = 3.20 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the aqueous-phase reaction with OH radical in solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{\text{OH}} = 4.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 5.79 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{\text{OH}} = (4.56 \pm 0.30) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ with calculated tropospheric lifetime $\tau = 2.5 \text{ d}$ (relative rate method, Atkinson et al. 2000)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 3.5 \text{ d}$ for reactions with photochemically produced OH radical (Howard 1990);

calculated lifetime $\tau = 2.5 \text{ d}$ for reaction with OH radical (Atkinson 2000).

Surface water: volatilization $t_{1/2} = 11\text{--}17 \text{ h}$ from a model river (Howard 1990).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.3.1

Reported aqueous solubilities of 2-pentanone at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	76406	20	59500	0	87000
30	54268	25	55100	9.7	69000
50	44362	30	51800	19.7	59000
				31.0	50000
		bp/°C	102.2–102.3	39.6	46000
		d ²⁵	0.8018	49.8	42000
				60.1	40000
				70.2	40000
				80.0	38000
				90.5	34000

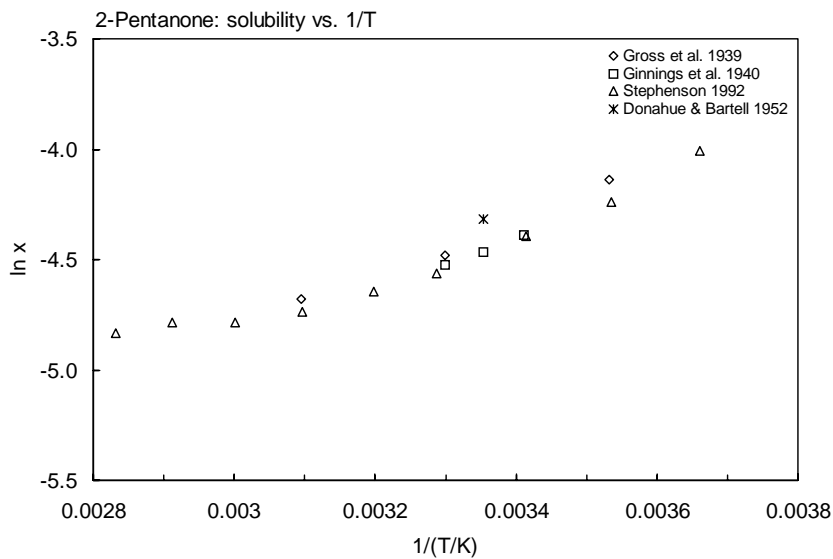


FIGURE 12.1.2.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-pentanone.

TABLE 12.1.2.3.2
Reported vapor pressures of 2-pentanone (methyl propyl ketone) at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K)$$
$$\log P = A - B/(C + t/^{\circ}\text{C})$$
$$\log P = A - B/(C + T/K)$$
$$\log P = A - B/(T/K) - C \cdot \log (T/K)$$

(1)

(2)

(3)

(4)

$$\ln P = A - B/(T/K)$$
$$\ln P = A - B/(C + t/^{\circ}\text{C})$$

(1a)

(2a)

Stull 1947		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−12.0	133.3	56.649	20440	63.175	26546
8	666.6	63.184	26546	68.889	33040
17.9	1333	68.897	33040	74.069	39992
28.5	2666	74.077	39991	78.333	46568
39.8	5333	78.34	46568	82.321	53466
47.3	7999	82.326	53466	85.703	59946
56.8	13332	85.708	59947	88.889	66611
71	26664	88.893	66527	91.832	73283
86.8	53329	91.834	73303	95.547	79906
103.3	101325	94.549	79905	97.178	86760
		97.179	86760	99.47	93107
mp/°C	−77.8	99.47	93107	101.845	100063
		101.345	100062	104.032	106831
		104.031	106831	106.116	113611
		106.114	113612	108.026	120112
		108.023	120113	109.834	126533
		109.83	126535	111.659	133292
		111.655	133283	25	4720
		mp/°C	−76.86	bp/°C	102.262
		bp/°C	102.26		

(Continued)

TABLE 12.1.2.3.2 (Continued)

Stull 1947		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		Antoine eq.		eq. 3	P/kPa
		eq. 2	P/mmHg	A	6.13925
		A	7.01753	B	1309.592
		B	1311.145	C	-58.589
		C	214.693		
		Kirchhoff eq		$\Delta H_v/(\text{kJ mol}^{-1}) =$	
		eq. 4	P/mmHg	at 25°C	38.4
		A	21.7188	at bp	33.6
		B	2594.12		
		C	4.63307		
		$\Delta H_v/(\text{kJ mol}^{-1}) = 33.64$			

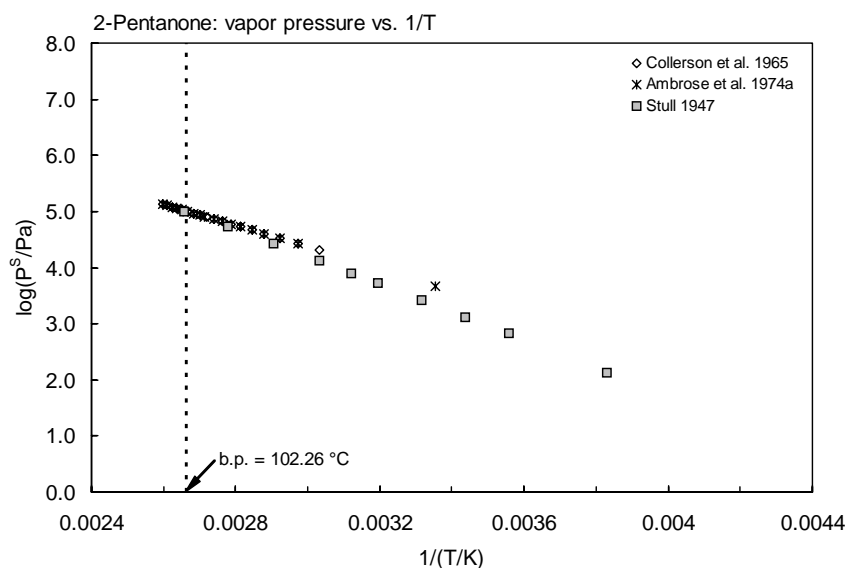
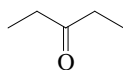


FIGURE 12.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for 2-pentanone.

12.1.2.4 3-Pentanone



Common Name: 3-Pentanone

Synonym: diethyl ketone, ethylketone, propione, *sym*-dimethylacetone

Chemical Name: 3-pentanone, diethyl ketone

CAS Registry No: 96-22-0

Molecular Formula: $C_5H_{10}O$, $CH_3CH_2COCH_2CH_3$

Molecular Weight: 86.132

Melting Point ($^{\circ}C$):

−39 (Lide 2003)

Boiling Point ($^{\circ}C$):

101.7 (Gross et al. 1933; Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8138 (Weast 1982–83)

0.8143, 0.8095 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.6 (calculated-density, Jaworska & Schultz 1993)

118.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

27.1 (pK_a , Riddick et al. 1986; Howard 1993)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

11.593 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

46900 ($30^{\circ}C$, shake flask-interferometer, Gross et al. 1933)

49617* ($30^{\circ}C$, shake flask-interferometer, measured range 10 – $50^{\circ}C$, Gross et al. 1939)

49620 ($30^{\circ}C$, shake flask-interferometer, Gross et al. 1933)

48100* (shake flask-volumetric method, measured range 20 – $30^{\circ}C$, Ginnings et al. 1940)

48100 (shake flask-volumetric, Ginnings et al. 1940)

44520 (shake flask-centrifuge, Booth & Everson 1948)

43170 (estimated, McGowan 1954)

47330 (Deno & Berkheimer 1960)

45650 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)

47000, 38000 ($20^{\circ}C$, $100^{\circ}C$, Verschuereen 1983)

34000 ($20^{\circ}C$, Riddick et al. 1986)

48440 (calculated-fragment solubility const., Wakita et al. 1986)

53000* ($19.3^{\circ}C$, shake flask-GC, measured range 0 – $80^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2169* (interpolated-regression of tabulated data, temp range -12.0 to $103.3^{\circ}C$, Stull 1947)

2666 ($27.9^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.25223 - 1450.0/(230 + t/^{\circ}C)$, (Antoine eq., Dreisbach & Martin 1949)

10114* ($36.36^{\circ}C$, ebulliometry, measured range 36.36 – $101.7^{\circ}C$, Dreisbach & Shrader 1949)

20441* ($56.649^{\circ}C$, ebulliometry, measured range 56.5 – $111.3^{\circ}C$, Collerson et al. 1965)

$\log(P/mmHg) = 7.027427 - 1309.655/(214.118 + t/^{\circ}C)$; temp range 56.5 – $111.3^{\circ}C$ (Antoine eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/mmHg) = 22.02258 - 2614.85/(T/K) - 4.72805 \cdot \log(T/K)$; temp range 56.5 – $111.3^{\circ}C$ (Kirchhoff eq., ebulliometric measurements, Collerson et al. 1965)

$\log(P/\text{mmHg}) = [-0.2185 \times 11183.0/(T/K)] + 9.406280$; temp range -12.7 – 102.7°C , (Antoine eq., Weast 1972–73)
 4723* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)
 1733 (20°C , Verschueren 1983)
 5316, 4714 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.1467 - 1307.941/(213.968 + t/^\circ\text{C})$, temp range 56.53 – 111.3°C (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.13703 - 1349.358/(224.351 + t/^\circ\text{C})$, temp range 36.36 – 101.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 4693 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.02529 - 1310.28/(214.19 + t/^\circ\text{C})$, temp range 56 – 111°C (Antoine eq., Dean 1985, 1992)
 4723 (Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 6.14917 - 1309.657/(-59.032 + T/K)$, temp range 329 – 384 K, (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.14635 - 1308.327/(-59.137 + T/K)$, temp range 329 – 426 K, (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.45505 - 1544.596/(-27.379 + T/K)$, temp range 421 – 502 K, (Antoine eq.-III, Stephenson & Malanowski 1987)
 4932 (Daubert & Danner 1989)
 $\log(P/\text{mmHg}) = 32.265 - 2.9431 \times 10^3/(T/K) - 8.5068 \cdot \log(T/K) - 4.572 \times 10^{-10} \cdot (T/K) + 2.5177 \times 10^{-6} \cdot (T/K)^2$;
 temp range 234 – 561 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

3.617 (calculated- γ -P, Rathbun & Tai 1982)
 5.340 (calculated-MW, Rathbun & Tai 1982)
 8.834 (calculated-P/C, Howard 1993)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.99 (generator column-GC, Wasik et al. 1981; Tewari et al. 1982)
 0.75 (calculated-activity coeff. γ , Wasik et al. 1981)
 0.67 (calculated- activity coeff. γ , Berti et al. 1986)
 1.15 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.82 (recommended, Sangster 1989, 1993)
 0.99 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.20 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

0.519 (estimated- K_{ow} , Lyman et al. 1990; quoted, Howard 1993)
 0.146 (estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{OC}$:

1.914 (soil, estimated- K_{ow} , Lyman et al. 1990; quoted, Howard 1993)
 1.08 (soil, estimated-S, Lyman et al. 1990; quoted, Howard 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated half-life from a model pond of two meter deep is 5.6 d (USEPA 1987; quoted, Howard 1993);
 based on calculated Henry's law constant, estimated $t_{1/2} \sim 12$ h from a model river of 1 m deep flowing at
 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3}
 with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:
 photooxidation $t_{1/2} = 2.4$ – 24 h for the gas-phase reaction with OH radical in air, based on the rate of
 disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = (1.82 \pm 0.33) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $299 \pm 2 \text{ K}$ in air (relative rate technique to cyclohexane Atkinson et al. 1982)

$k_{\text{OH}}(\text{calc}) = 2.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}}(\text{exptl}) = 2.74 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 296 K ; experimentally determined $k(\text{soln}) = 2.30 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington & Kurylo 1987; quoted, Wallington et al. 1988)

$k_{\text{OH}} = 2.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 3.23 \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: not expected to be important (Howard 1993).

Biodegradation: $t_{1/2} \sim 5$ to 10 d in acclimated cultures during screening tests (Howard 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photooxidation $t_{1/2} = 5.9 \text{ d}$, based on an experimentally determined rate constant for the vapor-phase reaction with OH radical in air (Wallington & Kurylo 1987; quoted, Howard 1993).

Surface water: estimated volatilization $t_{1/2} \sim 12 \text{ h}$ in a model river (1 m deep flowing at 1 m/s with a 3 m/s wind) and $t_{1/2} = 5.6 \text{ d}$ in a model environmental pond (2 m deep) (Howard 1993).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.4.1

Reported aqueous solubilities of 3-pentanone at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	67275	20	50800	0	76800
30	49617	25	48100	9.7	62500
50	39280	30	45000	19.3	53000
				30.6	42400
		bp/°C	101.6–101.9	40.3	38600
		D ²⁵	0.8116	50	36200
				60.1	34300
				70.1	33000
				80.2	31500

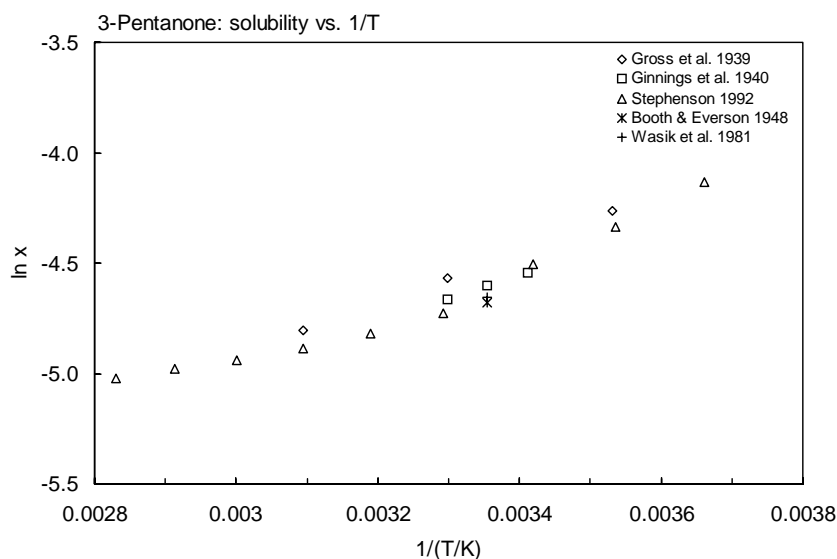


FIGURE 12.1.2.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-pentanone.

TABLE 12.1.2.4.2

Reported vapor pressures of 3-pentanone at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned} \log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log(T/K) & (4) & \end{aligned}$$

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
-12.7	133.3	36.36	10114	56.544	20441	56.534	20441
7.5	666.6	51.24	16500	63.032	26530	63.023	26529
17.2	1333	76.04	42066	68.735	33041	68.727	33041
27.9	2666	88.91	67661	73.908	40009	73.901	40009
39.4	5333	101.7	101325	78.158	46590	78.152	46589
46.7	7999			82.114	53473	82.109	53473
56.2	13332			85.494	59947	85.489	59979
70.6	26664			88.612	66532	88.608	66532
86.2	53329			91.605	74147	91.602	73348
102.7	101325			94.314	79985	94.312	79985
				96.897	86752	96.896	86752
mp/ $^{\circ}\text{C}$	-42			99.177	93092	99.176	93093
				101.566	100129	101.567	100129
				103.724	106835	103.725	106834
				105.737	113413	105.739	113412
				107.682	120061	107.685	120059
				109.486	126495	109.489	126493
				111.303	133254	111.307	133252
						25	4723
				mp/ $^{\circ}\text{C}$	-38.97		
				bp/ $^{\circ}\text{C}$	101.959	bp/ $^{\circ}\text{C}$	101.96

TABLE 12.1.2.4.2 (Continued)

Stull 1947		Dreisbach & Shrader 1949		Collerson et al. 1965		Ambrose et al. 1975(a)	
summary of literature data		ebulliometry		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				Antoine eq		eq. 3	P/kPa
				eq. 2	P/mmHg	A	6.1457
				A	7.02427	B	1307927
				B	1309.653	C	-59.184
				C	214.118		
				Kirchhoff eq. 4, P/mmHg		ΔH_v /(kJ mol ⁻¹) =	
				A	22.02258	at 25°C	38.6
				B	2614.85	at bp	33.7
				C	4.72085		
				ΔH_v /(kJ mol ⁻¹) = 33.72			

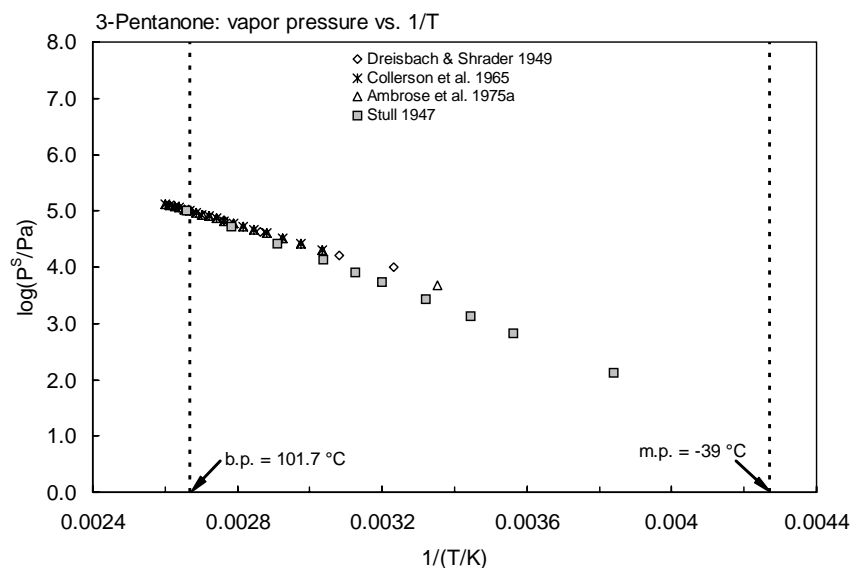
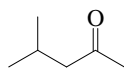


FIGURE 12.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for 3-pentanone.

12.1.2.5 Methyl isobutyl ketone (MIBK)



Common Name: Methyl isobutyl ketone

Synonym: hexone, hexanone, 4-methyl-2-pentanone, MIBK

Chemical Name: methyl isobutyl ketone, 4-methyl-2-pentanone

CAS Registry No: 108-10-1

Molecular Formula: $C_6H_{12}O$, $(CH_3)_2CHCH_2COCH_3$

Molecular Weight: 100.158

Melting Point ($^{\circ}C$):

-84 (Lide 2003)

Boiling Point ($^{\circ}C$):

116.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.7978 (Weast 1982-83)

0.8010 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

125.0 ($20^{\circ}C$, calculated-density)

140.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

16630* ($30^{\circ}C$, shake flask-interferometer, measured range $0-75^{\circ}C$, Gross et al. 1939)

19100* (shake flask-volumetric method, measured range $20-30^{\circ}C$, Ginnings et al. 1940)

19100 (shake flask-volumetric, Ginnings et al. 1940)

18200 (shake flask-turbidimeter, McBain & Richards 1946)

19085 (Deno & Berkheimer 1960)

17700 (shake flask-radiometric method, Lo et al. 1986)

17000 (Dean 1985; Riddick et al. 1986)

19200* ($19.4^{\circ}C$, shake flask-GC/TC, measured range $0-90.4^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* ($19.7^{\circ}C$, summary of literature data, temp range -1.40 to $119^{\circ}C$, Stull 1947)

2200* ($21.7^{\circ}C$, isoteniscope method, measured range $21.7-116.2^{\circ}C$, Fuge et al. 1952)

$\log (P/mmHg) = 31.1616 - 7.7701 \cdot \log (273.1 + t/^{\circ}C) - 3173.11/(273.11 + t/^{\circ}C)$; temp range $21.7-116.2^{\circ}C$ (isoteniscope method, Fuge et al. 1952)

$\log (P/mmHg) = [-0.2185 \times 11669.6/(T/K)] + 9.407655$; temp range: -1.4 to $119^{\circ}C$, (Antoine eq., Weast 1972-73)

800; 1333 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

2200 ($21.7^{\circ}C$, quoted exptl., Boublik et al. 1984; Howard 1990)

2587 (calculated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.81291 - 1176.833/(192.925 + t/^{\circ}C)$, temp range $21.7-116.2^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2575 (calculated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 6.6727 - 1168.4/(191.9 + t/^{\circ}C)$, temp range $22-116^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2510 (Riddick et al. 1986)

$\log (P/kPa) = 6.0976 - 1190.69/(195.45 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

2581, 2581 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.79768 - 1168.443/(-81.202 + T/\text{K})$, temp range 294–390 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 5.83311 - 1188.115/(-79.265 + T/\text{K})$, temp range 281–400 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

2687* (comparative ebulliometry, extrapolated-Antoine eq., measured range 309.7–416 K, Ambrose et al. 1988)

$\ln (p/\text{kPa}) = 14.07841 - 3103.029/(T/\text{K} - 61.104)$; temp range 309.7–416 K (comparative ebulliometry, Ambrose et al. 1988)

$\log (P/\text{mmHg}) = 64.1919 - 4.3577 \times 10^3/(T/\text{K}) - 19.766 \cdot \log (T/\text{K}) - 3.9997 \times 10^{-10} \cdot (T/\text{K}) + 7.102 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 189–571 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

39.5* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)

$\ln [H/(\text{atm m}^3/\text{mol})] = -7.157 + 160.6/(T/\text{K})$, temp range 10–30°C, (EPICS measurements, Ashworth et al. 1988)

9.523 (calculated-P/C, Howard 1990)

47.95* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)

$\ln (1/K_{AW}) = -9.56 + 4237/(T/\text{K})$, temp range: 40–80°C (equilibrium headspace-GC measurements, Kolb et al. 1992)

45.57 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996, 2001)

$\log K_{AW} = -1.924 + 57/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.38 (shake flask-GC, Iwasa et al. 1965)

1.09 (calculated- π constant, Hansch et al. 1968)

1.19 (Hansch & Leo, 1979)

1.39 (HPLC-RT correlation, Haky & Young 1984)

1.31 (shake flask-GC, Tanii et al. 1986)

1.38 (recommended, Sangster 1993)

1.31 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.301–0.699 (estimated- K_{OW} and S, Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.279–2.025 (soil, estimated- K_{OW} and S, Lyman et al. 1982; quoted, Howard 1990)

0.87 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 15\text{--}33$ h from water of 1 m deep, based on lab. mass-transfer coefficient for volatilization from a stirred 557–2020 rpm water bath at 25°C (Rathbun & Tai 1982; quoted, Howard 1990).

Photolysis: direct photolysis $t_{1/2} = 15$ h in air (Howard 1990).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 0.24\text{--}2.4$ h for the gas-phase reaction with OH radical in air, based on the disappearance rate of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (0.9 \pm 0.3) \times 10^{10} \text{ cm}^3 \text{ M}^{-1} \text{ s}^{-1}$ at 1 atm and 305 ± 2 K (relative rate method, Winer et al. 1976)

$k_{OH}(\text{calc}) = 9.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 14.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

photooxidation $t_{1/2} = 4.6\text{--}45.5$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991)

$k_{OH} = 14.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}} = (1.31 - 1.45) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (OH radical concn. of $8.0 \times 10^5 \text{ molecule}\cdot\text{cm}^{-3}$) at 22–27°C, estimated $t_{1/2} = 16\text{--}17 \text{ h}$ (Howard 1990)

$k_{\text{OH}}(\text{calc}) = 3.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: not expected to undergo chemical hydrolysis (Howard 1990).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic aqueous screening test data (Bridie et al. 1979; Takemoto et al. 1981; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 0.24\text{--}2.4 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the disappearance rate of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 3.5 \text{ h}$ under simulated atmospheric conditions, with NO (Dilling et al. 1976);

direct photolysis $t_{1/2} = 15 \text{ h}$ and photooxidation $t_{1/2} = 16\text{--}17 \text{ h}$ for reactions with hydroxyl radical in air (Howard 1990);

photooxidation $t_{1/2} = 4.6\text{--}45.5 \text{ h}$, based on measured rate data for the vapor phase reaction with hydroxyl radical (Atkinson 1985; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: estimated volatilization $t_{1/2} = 15\text{--}33 \text{ h}$ (Howard 1990);

$t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic aqueous biodegradation half-life (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 12.1.2.5.1

Reported aqueous solubilities of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	30749	10	20400	0	29200
10	23137	24	19100	9.5	22100
30	16630	30	17800	19.4	19200
50	14123			30.8	16600
75	13721	bp/ $^{\circ}\text{C}$	115.6–115.7	39.6	14700
		D ²⁵	0.7969	50.1	13800
				60.4	12900
				70.2	12400
				80.1	11800
				90.4	12200

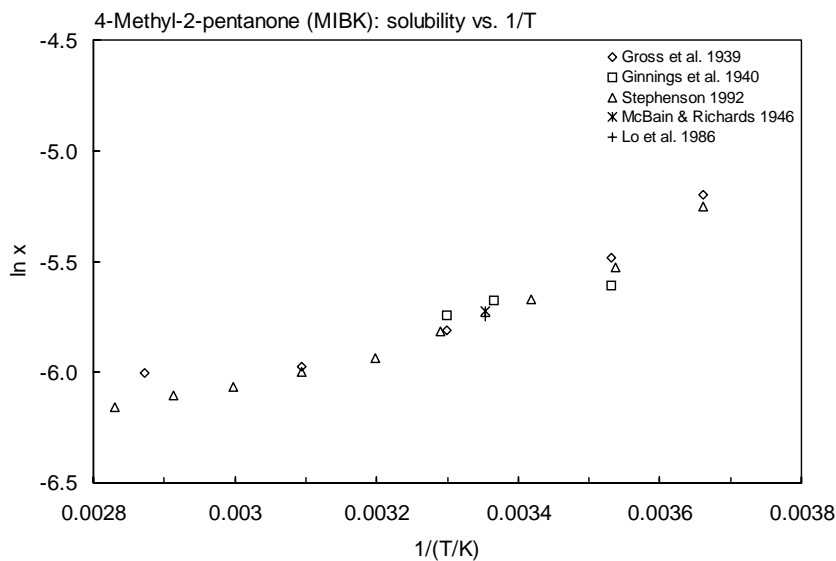


FIGURE 12.1.2.5.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-methyl-2-pentanone.

TABLE 12.1.2.5.2
Reported vapor pressures of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)
log P = A – B/(C + T/K)		(3)	ln P = A – B/(C + T/K)		(3a)
log P = A – B/(T/K) – C·log (T/K)		(4)			
Stull 1947		Fuge et al. 1952		Ambrose et al. 1988	
summary of literature data		isoteniscope method		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
–1.40	133.3	21.7	2200	309.676	4922
19.7	666.6	32.7	3933	314.495	6239
30.0	1333	41.4	6266	318.766	7638
40.8	2666	50.2	9266	324.624	9984
52.8	5333	60.0	14999	328.196	11607
60.4	7999	70.0	21598	334.215	15105
70.4	13332	80.1	31997	339.189	18512
85.6	26664	90.9	46396	343.458	21914
102.0	53329	116.2	101325	347.213	25314
119.0	101325			352.107	30381
		bp/K	389.35 K	359.039	38940
mp/°C	–84.7			365.854	49155
		eq. 4	P/mmHg	369.784	55938
		A	31.1616	373.360	62819
		B	3173.11	379.656	76425
		C	–7.7701	383.817	86848
				389.378	101960
				400.202	137928

(Continued)

TABLE 12.1.2.5.2 (Continued)

Stull 1947		Fuge et al. 1952		Ambrose et al. 1988	
summary of literature data		isoteniscope method		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
				408.620	172120
				415.823	206364
				298.15	2687
					(extrapolated)
				eq. 3a	P/kPa
				A	14.07841
				B	3103.029
				C	-61.104

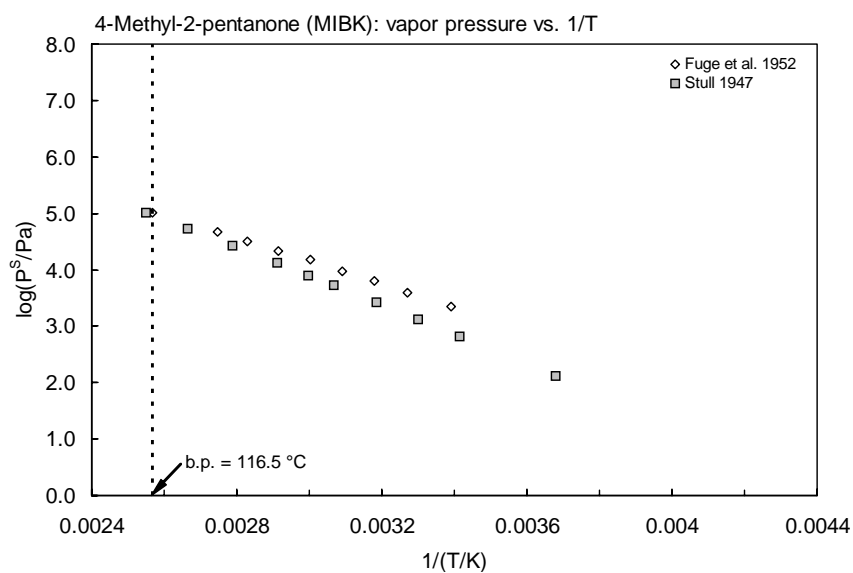


FIGURE 12.1.2.5.2 Logarithm of vapor pressure versus reciprocal temperature for 4-methyl-2-pentanone.

TABLE 12.1.2.5.3
Reported Henry’s law constants of 4-methyl-2-pentanone (methyl isobutyl ketone) at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln [H/(\text{Pa m}^3/\text{mol})] = A - B/(T/K)$		(4)	$\ln [H/(\text{atm}\cdot\text{m}^3/\text{mol})] = A - B/(T/K)$		(4a)
$K_{AW} = A - B\cdot(T/K) + C\cdot(T/K)^2$		(5)			
Ashworth et al. 1988			Kolb et al. 1992		
EPICS-GC			equilibrium headspace-GC		
t/°C	H/(Pa m³/mol)		t/°C	H/(Pa m³/mol)	
10	66.87		40	47.95	
15	37.49		60	121.5	
20	29.38		70	176	
25	39.52		80	248.8	
30	68.90				
			eq. 2	1/K _{AW}	
			A	−9.56	
eq. 4a	H/(atm·m ³ /mol)		B	4237	
A	−7.157				
B	160.6				

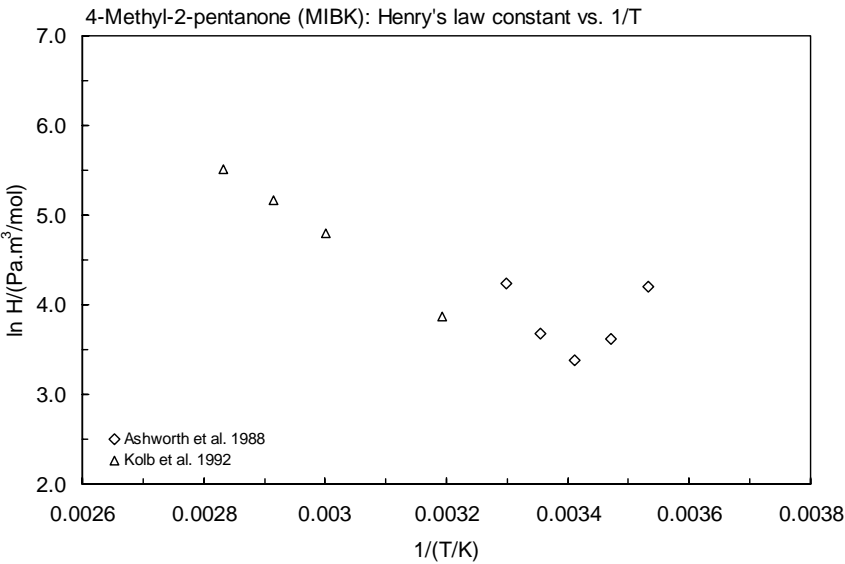
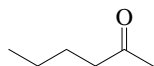


FIGURE 12.1.2.5.3 Logarithm of Henry’s law constant versus reciprocal temperature for 4-methyl-2-pentanone.

12.1.2.6 2-Hexanone (Methyl butyl ketone)



Common Name: Methyl butyl ketone

Synonym: 2-hexanone, methyl *n*-butyl ketone

Chemical Name: 2-hexanone, methylbutyl ketone

CAS Registry No: 591-78-6

Molecular Formula: $C_6H_{12}O$, $CH_3COCH_2CH_2CH_2CH_3$

Molecular Weight: 100.158

Melting Point ($^{\circ}C$):

-55 (Lide 2003)

Boiling Point ($^{\circ}C$):

127.6 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8113 (Weast 1982-83)

0.8113, 0.8067 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

124.2 (calculated-density, Hoy 1970; Amidon & Williams 1982)

140.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

-8.30 (pK_a , Riddick et al. 1986)

25.30 (pK_s , Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

3.56 (Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

14523* ($30^{\circ}C$, shake flask-interferometer, measured range $10-50^{\circ}C$, Gross et al. 1939)

16400* (shake flask-volumetric method, measured range $20-30^{\circ}C$, Ginnings et al. 1940)

16400 (shake flask-volumetric, Ginnings et al. 1940)

16000 (Erichsen 1952)

23930 (shake flask-interferometer, Donahue & Bartell 1952)

15870 (estimated, McGowan 1954)

16620 (Deno & Berkheimer 1960)

35000 ($20^{\circ}C$, Verschueren 1983)

17500 ($20^{\circ}C$, Riddick et al. 1986)

15100*, 13700 ($19.8^{\circ}C$, $29.7^{\circ}C$, shake flask-GC, measured range $0-91.5^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

514.4* (interpolated-regression of tabulated data, temp range $7.7-212.6^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 12358.3/(T/K)] + 9.642791$; temp range $7.7-127.5^{\circ}C$, (Antoine eq., Weast 1972-73)

1549* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)

509.8 (calculated-Cox eq., Chao et al. 1983)

266.6 ($20^{\circ}C$, Verschueren 1983)

1540 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.15217 - 1395.406/(208.946 + t/^{\circ}C)$, temp range $34.61-154.6^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

1549 (Riddick et al. 1986)

$\log(P/kPa) = 6.16230 - 1401.738/(209.646 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

1715, 1540 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.4127 - 1575.5/(-43.15 + T/\text{K})$, temp range 293–411 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.14816 - 1392.968/(-64.465 + T/\text{K})$, temp range 279–423 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15949 - 1399.959/(-63.704 + T/\text{K})$, temp range 310–427 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

1600 (computed-expert system SPARC, Kolling 1995)

$\log (P/\text{mmHg}) = 4.0508 - 2.6276 \times 10^3/(T/\text{K}) + 3.7783 \cdot \log (T/\text{K}) - 1.4342 \times 10^{-2} \cdot (T/\text{K}) + 8.0592 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 217–587 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$):

9.69 (calculated-P/C, Meylan & Howard 1991)

11.8 (calculated-bond contribution, Meylan & Howard 1991)

9.70 (calculated-P/C, Howard 1993)

8.82 (computed-expert system SPARC, Kolling 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.38 (shake flask-UV, Iwasa et al. 1965; Leo et al. 1971; Hansch & Leo 1979)

1.29 (calculated- π constant, Hansch et al. 1968)

1.39 (HPLC- k' correlation, Haky & Young 1984)

1.19 (shake flask-GC, Tanii et al. 1986)

1.38 (recommended, Sangster 1989, 1993)

1.38 (recommended, Hansch et al. 1995)

1.30 (computed-expert system SPARC, Kolling 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

3.68 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

0.778 (estimated- K_{OW} , Lyman et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

1.322 (soil, estimated- K_{OW} , Lyman et al. 1990)

2.127 (soil, estimated-S, Lyman et al. 1990)

1.10 (computed- K_{OW} , Kolling 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 135$ h from a model environmental pond of 2 m deep (USEPA 1987; quoted, Howard 1993); using Henry's law constant, $t_{1/2} \sim 12.1$ H from a model river of 1 m deep flowing at 1 m/s with a wind speed of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (6.81 \pm 0.29) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(299 \pm 2) \text{ K}$ (relative rate technique to cyclohexane, Atkinson et al. 1982; quoted, Atkinson 1985)

$k_{OH}(\text{calc}) = 7.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 8.97 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH} = 9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH} = 9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C, which corresponds to a half-life of 42 h at an atmospheric OH- concn of $5 \times 10^5 \text{ molecule cm}^{-3}$ (quoted, Howard 1993)

$k_{OH}(\text{calc}) = 10.57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: half-life of approximately 5 d in acclimated mixed microbial culture (Howard 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

estimated $t_{1/2} \sim 42$ h for the vapor-phase reaction with OH radical is 42 h at an atmospheric OH- concentration of 5×10^5 molecule·cm⁻³ (Atkinson 1985; quoted, Howard 1993).

Surface water: volatilization $t_{1/2} = 12.1$ h from a model river, 135 h from a model environmental pond (Howard 1993).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.6.1

Reported aqueous solubilities of 2-hexanone at various temperatures

Gross et al. 1939		Ginnings et al. 1940		Stephenson 1992	
shake flask-IR		volumetric method		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
10	20433	20	17500	0	24600
30	14523	25	16400	9.6	19100
50	12420	30	15300	19.8	15100
				29.7	13700
		bp/°C	127.5–127.6	39.6	12400
		d ²⁵	0.8072	50.0	11600
				60.5	11200
				70.3	11200
				80.7	11500
				91.5	11900

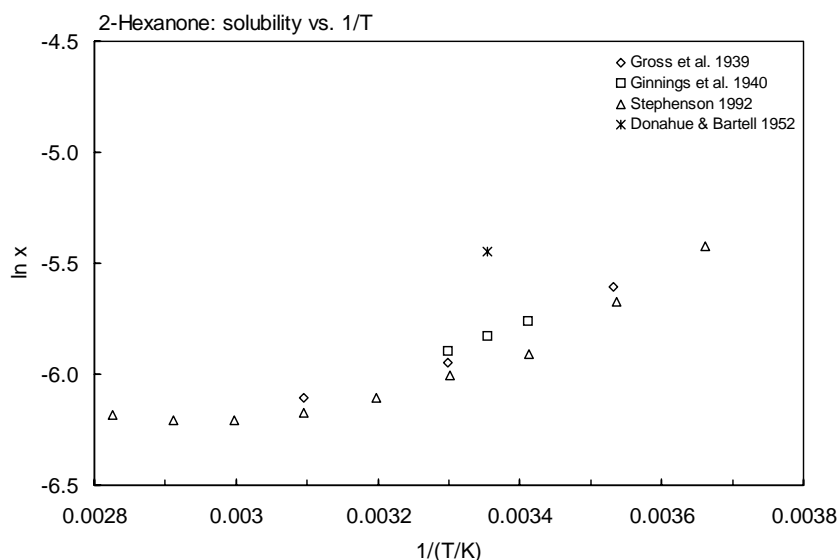


FIGURE 12.1.2.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-hexanone.

TABLE 12.1.2.6.2

Reported vapor pressures of 2-hexanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Ambrose et al. 1975(a)			
summary of literature data		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
7.7	133.3	34.612	2656	cont'd	
28.8	666.6	37.070	3024	128.935	105328
38.8	1333	41.117	3737	133.789	120447
50.0	2666	44.498	4434	138.034	135072
62.0	5333	48.033	5277	143.528	156043
69.8	7999	51.799	6319	149.390	181140
79.8	13332	55.414	7476	154.613	206034
94.3	26664	59.402	8955	25.0	1549
111.0	53329	63.784	10853	bp/°C	127.583
127.5	101325	67.976	12972		
mp/°C	−56.9	72.537	15657	Antoine eq. for full range:	
		77.315	18944	eq. 3	P/kPa
		82.256	22918	A	6.16230
		86.138	26494	B	1401.738
		91.579	32278	C	−63.504
		96.410	38230	$\Delta H_v/(\text{kJ mol}^{-1}) =$	
		101.664	45683	at 25°C	42.9
		106.935	54287	at bp	36.0
		112.320	64383	Antoine eq. for restricted range of	
		117.459	75365	of atmospheric pressure:	
		122.839	88399	eq. 3	P/kPa
		127.231	100312	A	6.14801
		127.653	101527	B	1392.870
		128.362	103586	C	−64.477

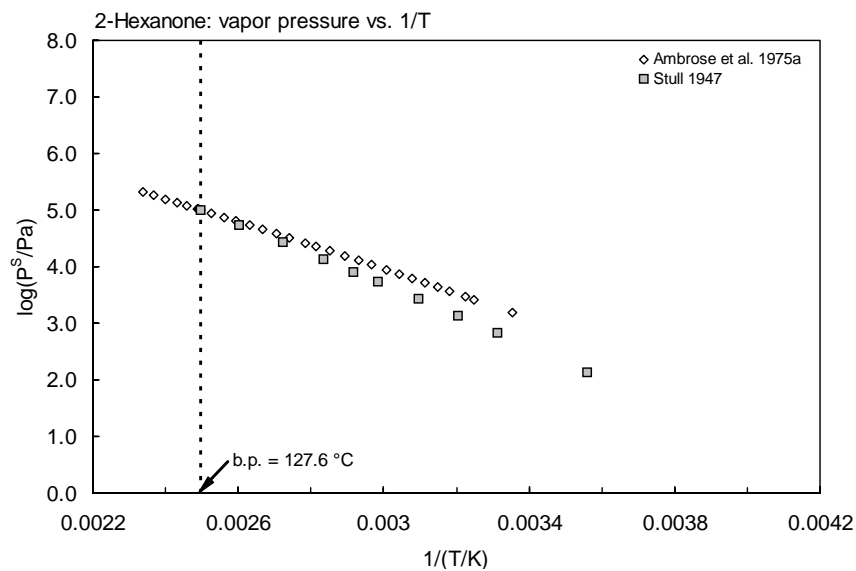
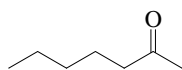


FIGURE 12.1.2.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2-hexanone.

12.1.2.7 2-Heptanone



Common Name: 2-Heptanone

Synonym: methyl *n*-amyl ketone, methyl pentyl ketone

Chemical Name: 2-heptanone

CAS Registry No: 110-43-0

Molecular Formula: $C_7H_{14}O$, $CH_3(CH_2)_4COCH_3$

Molecular Weight: 114.185

Melting Point ($^{\circ}C$):

−35 (Lide 2003)

Boiling Point ($^{\circ}C$):

151.05 (Lide 2003)

Density (g/cm^3):

0.81537, 0.81123 (20 $^{\circ}C$, 25 $^{\circ}C$, Riddick et al. 1986)

Dissociation Constant:

Molar Volume (cm^3/mol):

141.5 (30 $^{\circ}C$, Stephenson & Malanowski 1987)

162.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

4300* (25 $^{\circ}C$, volumetric method, measured range 20–30 $^{\circ}C$, Ginnings et al. 1940)

4054* (30 $^{\circ}C$, shake flask-interferometer, measured range 10–75 $^{\circ}C$, Saylor et al. 1942)

4546 (estimated, McGowan 1954)

4300 (Riddick et al. 1986)

4360* (19.7 $^{\circ}C$, shake flask-GC/TC, measured range 0–90.5 $^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

521 (interpolated-vapor pressure eq., temp range 4–75 $^{\circ}C$, Stuckey & Saylor 1940)

$\log (P/mmHg) = 7.36537 - 1650.47/(T/K - 54.48)$; temp range 4–75 $^{\circ}C$ (Antoine eq., Ramsay-Young method-Hg manometer, Stuckey & Saylor 1940)

709* (30 $^{\circ}C$, measured range 10–75 $^{\circ}C$, Saylor et al. 1942)

133.3* (19.3 $^{\circ}C$, summary of literature data, temp range 19.3–150.2 $^{\circ}C$, Stull 1947)

$\log (P/mmHg) = 5.95166 - 1408.13/(194.84 + t/^{\circ}C)$; temp range 36 to 151 $^{\circ}C$ (data fitted to Antoine eq., static method-Ramsay-Young apparatus measurements, Meyer & Wagner 1966)

$\log (P/mmHg) = [-0.2185 \times 12478.9/(T/K)] + 9.305642$, temp range 19.3–150.2 $^{\circ}C$, (Antoine eq., Weast 1972–73)

427* (ebulliometry-fitted to Antoine eq., Ambrose et al. 1975a)

$\log (P/mmHg) = [1 - 400.348/(T/K)] \times 10^4 \{0.934881 - 4.87941 \times 10^{-4} \cdot (T/K) + 4.16258 \times 10^{-7} \cdot (T/K)^2\}$; temp range 280.85–400.65 K, (Cox eq., Chao et al. 1983)

514 (Abraham 1984; Riddick et al. 1986)

504 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.14611 - 1460.276/(201.636 + t/^{\circ}C)$, temp range 94.7–179.3 $^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1975, Boublik et al. 1984)

469 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.07656 - 1408.73/(-78.31 + T/K)$, temp range 303–424 K, (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.15178 - 1464.092/(-71.076 + T/\text{K})$, temp range 327–457 K, (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.56718 - 1810.283/(-26.944 + T/\text{K})$, temp range 449–580 K, (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -13.0256 - 2.6425 \times 10^3/(T/\text{K}) + 11.879 \cdot \log (T/\text{K}) - 2.7571 \times 10^{-2} \cdot (T/\text{K}) + 1.456 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 238–612 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

14.63 (partial vapor pressure-GC, Buttery et al. 1969)

14.6; 14.94, 14.6 (exptl.; calculated-group contribution, bond contribution, Hine & Mookerjee 1975)

5.715 (calculated-activity coefficient γ_P , Rathbun & Tai 1982)

9.120 (calculated-P/C, Mackay & Yuen 1983)

16.0 (correlated-molecular structure, Russell et al. 1992)

17.1 (gas stripping-GC, Shiu & Mackay 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.08 (calculated-activity coefficients, Wasik et al. 1981)

1.98 (generator column-HPLC, Tewari et al. 1982)

2.00 (shake flask-GC, Tani et al. 1986)

2.03 (calculated-UNIFAC activity coefficients, Dallos et al. 1993)

1.98 (recommended, Sangster 1993)

1.98 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

4.15 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (8.67 \pm 8.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Wallington et al. 1987; quoted, Atkinson 1989)

$k_{OH}(\text{calc}) = 13.10 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

$k_{OH} = (1.17 \pm 0.11) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 2 \text{ K}$ with calculated tropospheric lifetime $\tau = 1.0 \text{ d}$ (relative rate method, Atkinson et al. 2000)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime $\tau = 1.0 \text{ d}$, based on gas-phase reaction with OH radical (relative rate method, Atkinson et al. 2000)

Surface water:

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.7.1

Reported aqueous solubilities of 2-heptanone at various temperatures

Ginnings et al. 1940		Saylor et al. 1942		Stephenson 1992	
volumetric method		shake flask-interferometer		shake flask-GC/TC	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
20	4400	10	5390	0	6490
25	4300	30	4054	9.7	5350
30	4000	50	3643	19.8	4360
		60	3517	30.7	3580
bp/°C	151.2–151.3	65	3597	39.7	3430
d ²⁵	0.8115	75	3871	49.8	3360
				60.2	3330
				70.1	3140
				80.2	3480
				90.5	3530

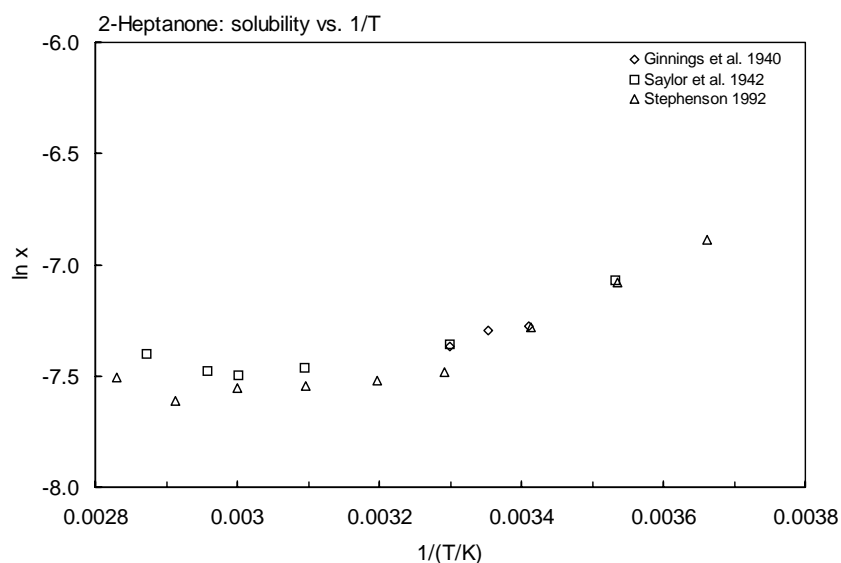
FIGURE 12.1.2.7.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-heptanone.

TABLE 12.1.2.7.2

Reported vapor pressures of 2-heptanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stuckey & Saylor 1940		Stull 1947		Ambrose et al. 1975(a)			
static method-Hg manometer		summary of literature data		comparative ebulliometry			
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
						cont'd	
data presented as		19.3	133.3	54.687	2818	151.949	103789
eq. 3	P/mmHg	43.5	666.6	57.076	3180	157.300	119605
A	7.36537	55.5	1333	60.142	3697	162.280	136005
B	1650.47	67.7	2666	64.213	4500	168.137	157388
C	-54.48	81.2	5333	67.814	5324	173.697	180116
		89.8	7999	71.989	6433	179.267	205316
		100.0	13332	71.991	6436	25.0	427
		116.1	26664	75.736	7617		
Saylor et al. 1942		133.2	53329	79.945	9127	bp/ $^{\circ}\text{C}$	151.058
Stuckey & Saylor data		150.2	101325	84.035	10826		
10	188	mp/ $^{\circ}\text{C}$	-	88.302	12873	Antoine eq. for full range:	
30	709			92.564	15282	eq. 3	P/kPa
50	1973			95.832	17932	A	6.15034
60	3733			102.322	21975	B	1462.981
65	4720			107.012	25997	C	-71.24
75	7413			112.377	31321	$\Delta H_{\text{V}}/(\text{kJ mol}^{-1}) =$	
				117.486	37167	at 25 $^{\circ}\text{C}$	38.3
				117.629	37361	at bp	33.2
				123.186	44713		
				129.297	54129	Antoine eq. for restricted	
				134.589	63526	range of atm. pressure:	
				140.221	74904	eq. 3	P/kPa
				146.323	88989	A	6.15033
				150.976	101114	B	1463.072
						C	-71.200

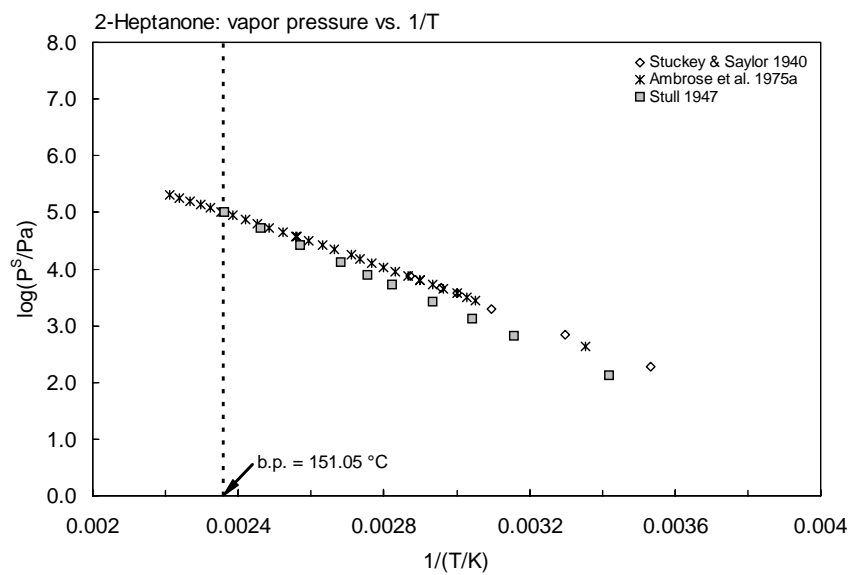
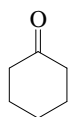


FIGURE 12.1.2.7.2 Logarithm of vapor pressure versus reciprocal temperature for 2-heptanone.

12.1.2.8 Cyclohexanone



Common Name: Cyclohexanone

Synonym:

Chemical Name: cyclohexanone

CAS Registry No: 108-94-1

Molecular Formula: C₆H₁₀O

Molecular Weight: 98.142

Melting Point (°C):

-27.9 (Lide 2003)

Boiling Point (°C):

155.43 (Lide 2003)

Density (g/cm³ at 20°C):

0.9478 (Weast 1982-83; Dean 1985)

0.9452 (Riddick et al. 1986)

Molar Volume (cm³/mol):

106.2 (calculated-density, Stephenson & Malanowski 1987)

118.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56$ J/mol K, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

23000 (Riddick et al. 1986)

93200 (selected, Yaws et al. 1990)

97000*, 82000 (19.5°C, 29.8°C, shake flask-GC, measured range 0-90.7°C, Stephenson 1992)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* (26.4°C, summary of literature data, temp range 1.4-155.6°C, Stull 1947)

$\log(P/\text{mmHg}) = [-0.2185 \times 10037.6/(T/K)] + 8.019908$; temp range 1.4-155.6°C, (Antoine eq., Weast 1972-73)

533* (ebulliometry-fitted to Antoine eq., temp range 89.6-165.8°C, Meyer & Hotz 1973)

$\log(P/\text{mmHg}) = 5.978401 - 1495.511/(209.5517 + t/^\circ\text{C})$; temp range 89.6-165.8°C (Antoine eq. ebulliometric measurements, Meyer & Hotz 1973)

614 (interpolated-Cox eq., Chao et al. 1983)

$\log(P/\text{mmHg}) = [1 - 428.587/(T/K)] \times 10^{0.833332 - 6.42578 \times 10^{-4} \cdot (T/K) + 7.09855 \times 10^{-7} \cdot (T/K)^2}$; temp range: 274.55-438.92 K (Cox eq., Chao et al. 1983)

533 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.10133 - 1494.166/(209.399 + t/^\circ\text{C})$, temp range 89.29-165.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

640 (Riddick et al. 1986)

$\log(P/\text{kPa}) = 6.103304 - 1495.511/(209.5517 + t/^\circ\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)

620, 534 (calculated-Antoine eq.-I, extrapolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_s/\text{kPa}) = 8.434 - 2576.6/(T/K)$; temp range not specified (Antoine eq., solid, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.103304 - 1495.511/(-63.5983 + T/K)$, temp range 362-439 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 70.5022 - 4.412 \times 10^3/(T/K) - 23.605 \cdot \log(T/K) + 1.1205 \times 10^{-2} \cdot (T/K) - 1.5648 \times 10^{-13} \cdot (T/K)^2$; temp range 242-629 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

1.216	(Hawthorne et al. 1985)
2.266	(calculated-P/C, Meylan & Howard 1991)
5.179	(estimated-bond contribution, Meylan & Howard 1991)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.81	(shake flask, Hansch & Leo 1979, 1985, 1987)
0.81	(recommended, Sangster 1989, 1993)
0.81	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

0.39	(calculated- K_{OW} with regression eq., Lyman et al. 1982; quoted, Howard 1990)
------	---

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.00	(calculated-S, K_{OW} with regression eq., Roy & Griffin 1985; quoted, Howard 1990)
------	--

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 3.1$ d from a model river 1-m deep flowing 1 m s^{-1} with wind velocity of 3 m s^{-1} (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: direct sunlight photolysis rate constant of about 0.16 d^{-1} corresponding to $t_{1/2} = 4.3$ d (Mill & Davenport 1986; quoted, Howard 1990).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with OH radical, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = 1.56 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} \sim 1$ d (Atkinson 1985; quoted, Howard 1990)

$k_{\text{OH}} = 6.39 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{\text{OH}} = 12.55 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ from Atmospheric Oxidation Program, $k_{\text{OH}}(\text{exptl}) = 6.39 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{OH}}(\text{calc}) = 2.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ from Fate of Atmospheric Pollutants Program, (Meylan & Howard 1993)

$k_{\text{OH}}(\text{calc}) = 5.09 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation: average rate of biodegradation $51.5 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 24$ h to 9.9 d in air for the gas-phase reaction with hydroxyl radicals, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976);
degrade rapidly by reaction with sunlight produced hydroxyl radicals with $t_{1/2} \sim 1$ d and by direct sunlight photolysis with $t_{1/2} \sim 4.3$ d (Howard 1990).

Surface water: estimated $t_{1/2} \sim 0.003$ yr at Noordwijk (Zoeteman et al. 1981).

Ground water:

Sediment:

Soil:

Biota:

TABLE 12.1.2.8.1

Reported vapor aqueous solubilities and vapor pressures of cyclohexanone at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
$\log (P/\text{atm}) = A'[1 - (T_{\text{B}}/T)]$		(5)	where $A' = (a + bT + cT^2)$		
Aqueous solubility		Vapor pressure			
Stephenson 1992		Stull 1947		Meyer & Hotz 1973	
shake flask-GC/TC		summary of literature data		comparative ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
0	137000	1.40	133.3	89.628	12725
9.8	115000	26.4	666.6	94.986	15528
19.5	97000	38.7	1333	100.807	19257
29.8	82000	52.5	2666	107.664	24477
40.1	75000	67.8	5333	114.303	30580
50.2	70000	77.5	7999	119.712	36416
60.5	67000	90.4	13332	125.282	43337
71.1	65000	110.3	26664	130.659	50990
80.2	68000	132.5	53329	135.774	59239
90.7	69000	155.6	101325	141.742	70181
				145.880	78656
		mp/°C	−45.0	151.916	92474
				151.969	92593
				156.917	105300
				156.988	105417
				165.769	131422
				bp/°C	155.422
				Antoine eq.	
				eq. 2	P/cmHg
				A	5.978401
				B	1495.511
				C	209.5517
				Cox eq.	
				eq. 5	P/atm
				a	0.852046
				−b × 10 ³	0.612660
				c × 10 ⁶	0.504661
				T _B /K	428.5716

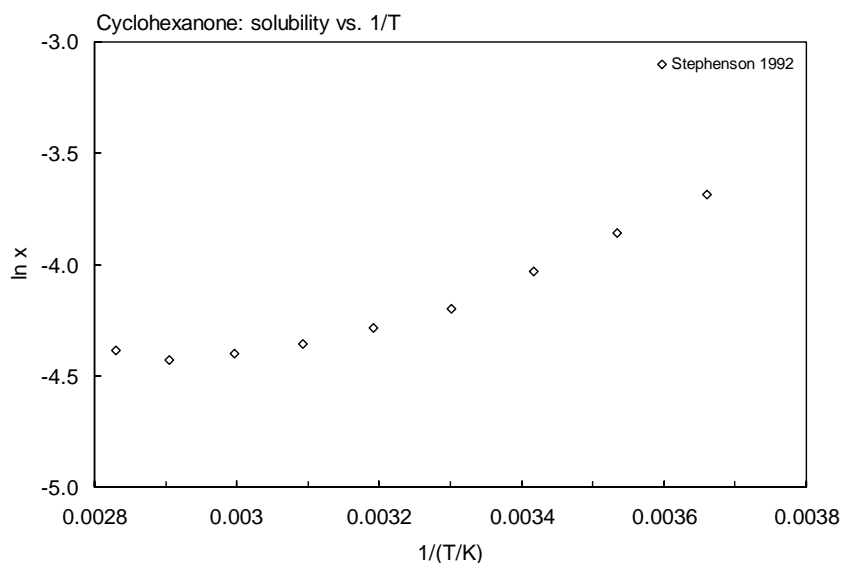


FIGURE 12.1.2.8.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for cyclohexanone.

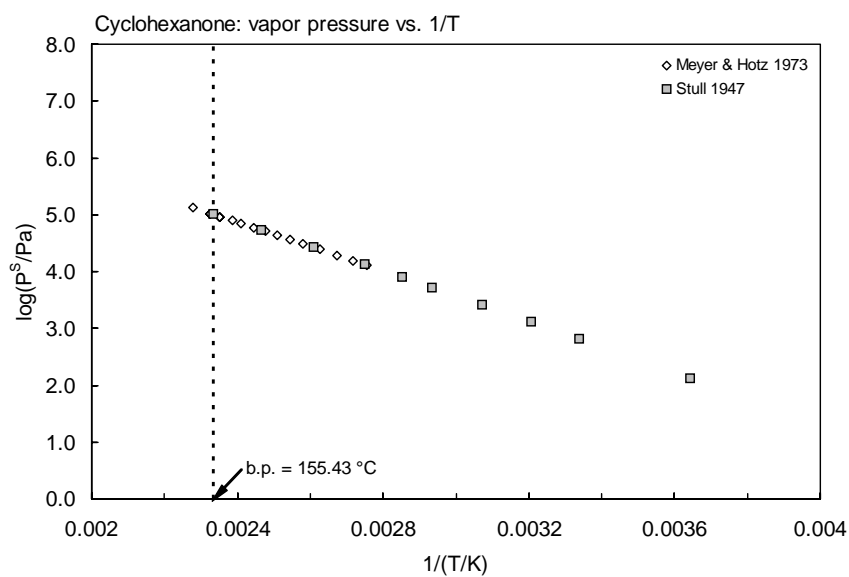
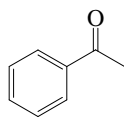


FIGURE 12.1.2.8.2 Logarithm of vapor pressure versus reciprocal temperature for cyclohexanone.

12.1.2.9 Acetophenone



Common Name: Acetophenone

Synonym: 1-phenylethanone, methyl phenyl ketone, acetylbenzene, phenylmethylketone, hypnone

Chemical Name: acetophenone, methyl phenyl ketone

CAS Registry No: 98-86-2

Molecular Formula: C_8H_8O , $C_6H_5COCH_3$

Molecular Weight: 120.149

Melting Point ($^{\circ}C$):

20.5 (Stull 1947; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

202 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0281 (Dreisbach 1955; Weast 1982–83; Riddick et al. 1986)

1.02382 ($25^{\circ}C$, Dreisbach 1955; Riddick et al. 1986)

Molar Volume (cm^3/mol):

117.1 (calculated-density, Rohrschneider 1973)

140.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

42.0, 53.41 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

16.65 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

42.26 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5530 (shake flask-centrifuge, Booth & Everson 1948)

6300 (shake flask-UV, Andrews & Keefer 1950)

6022 (estimated, McGowan 1954)

5540 ($24^{\circ}C$, shake flask-LSC, Means et al. 1980)

5500 (Verschueren 1983; Dean 1985, 1992)

6130 (Southworth & Keller 1986)

5620* ($19.9^{\circ}C$, shake flask-GC/TC, measured range 19.9 – $80.1^{\circ}C$, Stephenson 1992)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

266.6* ($50.2^{\circ}C$, static method-manometer, measured range 50.2 – $201.5^{\circ}C$, Kahlbaum 1898)

66.21* (extrapolated-regression of tabulated data, temp range 37.1 – $202.4^{\circ}C$, Stull, 1947)

49.53 (calculated-Antoine eq., Dreisbach 1955)

$\log (P/mmHg) = 7.15738 - 1723.46/(201.0 + t/^{\circ}C)$; temp range 102 – $330^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

41.30 (Hoy 1970)

$\log (P/mmHg) = [-0.2185 \times 11731.5/(T/K)] + 8.293248$; temp range 37.1 – $202.4^{\circ}C$ (Antoine eq., Weast 1972–73)

57.48 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/mmHg) = [1 - 474.823/(T/K)] \times 10^{0.859974 - 6.15392 \times 10^{-4} \cdot (T/K) + 6.99110 \times 10^{-7} \cdot (T/K)^2}$; temp range 310.25 – $475.55 K$ (Cox eq., Chao et al. 1983)

52.92 (Daubert & Danner 1985)

40.23 (extrapolated-Antoine eq., Dean 1985)

- log (P/mmHg) = $9.1352 - 2878.8/(T/K)$; temp range 20–100°C (Antoine eq., Dean 1985, 1992)
 49.0 (Riddick et al. 1986)
 log (P/kPa) = $6.28228 - 1723.46/(201.0 + t/^{\circ}\text{C})$, temp range not specify (Antoine eq., Riddick et al. 1986)
 45.3 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 log (P_L /kPa) = $6.28228 - 1723.46/(-72.15 + T/K)$; temp range 375–603 K (Antoine eq., Stephenson & Malanowski 1987)
 45.00 (selected, Mackay et al. 1992, 1995; quoted, Shiu & Mackay 1997)
 log (P/mmHg) = $55.5798 - 4.5101 \times 10^3/(T/K) - 17.284 \cdot \log (T/K) + 6.4184 \times 10^{-3} \cdot (T/K) + 6.5557 \times 10^{-13} \cdot (T/K)^2$;
 temp range 293–701 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.082 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)
 0.784 (calculated-bond contribution, Hine & Mookerjee 1975)
 0.921* (25.1°C, gas stripping-GC, measured range 14.9–35°C, Betterton 1991)
 0.753 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 1.080, 0.982 (gas stripping-GC, calculated-P/C, Shiu & Mackay 1997)
 1.06* (EPICS-UV spectroscopy, measured range 5–25°C, Allen et al. 1998)
 $\ln K_{AW} = -9100/(T/K) + 22.47$ (EPICS-UV, temp range 5–25°C, Allen et al. 1998)
 0.560 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 7.307 - 3202/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, log K_{OW} :

- 1.58 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1969, 1971; Hansch & Leo 1985)
 1.58 (calculated- π const., Iwasa et al. 1965)
 1.73 (shake flask-UV, Chapman et al. 1972)
 1.58 (HPLC-RT correlation, Lazare et al. 1974)
 1.68 (shake flask-UV, Holmes & Lough 1976)
 1.66 ± 0.08 (shake flask at pH 7, Unger et al. 1978)
 1.66 (Hansch & Leo 1979)
 1.59 (shake flask-GC, Khan et al 1979)
 1.59 (shake flask-LSC, Means et al. 1980)
 1.58 (shake flask-HPLC, Nahum & Horvath 1980)
 1.75 (calculated-f const., Rekker's method, Hanai et al. 1981)
 1.77, 1.56 (HPLC- k' correlation, McDuffie 1981)
 1.80 (HPLC-RT correlation, Hammers et al. 1982)
 1.83 (RP-LC-RT correlation, Hanai & Hubert 1982)
 1.56 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.63 (inter-laboratory studies, shake flask average, Eadsforth & Moser 1983)
 1.65 (inter-laboratory studies, HPLC average, Eadsforth & Moser 1983)
 1.65; 1.68 ± 0.02 (selected best lit. value; exptl.-ALPM, Garst & Wilson 1984)
 1.59; 1.72 (HPLC-RT correlation; HPLC average, Eadsforth 1986)
 1.71 (HPLC-RT correlation, Ge et al. 1987)
 1.65 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 1.60 (shake flask-CPC, Berthod et al. 1988)
 1.58 (RP-HPLC- k' correlation, Minick et al. 1988)
 1.63 (recommended, Sangster 1989, 1993)
 1.59 (CPC centrifugal partition chromatography, Gluck & Martin 1990)
 1.56 (shake flask-UV spec., Alcorn et al. 1993)
 1.58 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 0.699–0.954 (estimated- K_{OW} and S, Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, log K_{OC} :

- 1.544 (average of 3 sediments and soil samples, equilibrium sorption isotherm, Means et al. 1980)
- 1.380 (calculated, Means et al. 1980)
- 1.89 (calculated-MCI χ , Gerstl & Helling 1987)
- 1.630 (soil, quoted, Sabljic 1987)
- 1.73 (RP-HPLC- k' correlation, cyanopropyl column, Hodson & Williams 1988)
- 1.34–2.43 (soils and sediments, quoted exptl. and estimated values, Howard 1993)
- 1.26 (calculated- K_{OW} , Kollig 1993)
- 1.54 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.79, 1.63 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
- 1.61, 1.50, 1.80 (soils: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, $0.1 \leq \text{OC} < 0.5\%$, average, Delle Site 2001)
- 1.56, 1.55 (sediments: organic carbon OC $\geq 0.1\%$, OC $\geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on calculated Henry's law constant, $t_{1/2} \sim 3.8$ d from a model river of 1-m deep flowing at 1 m s^{-1} with a wind velocity of 3 m s^{-1} (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$$k_{OH} = (2.74 \pm 0.15) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K (Atkinson 1989)}$$

$k_{OH}(\text{calc}) = 1.61 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Atmospheric Oxidation Program; $k_{OH}(\text{exptl}) = 2.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Fate of Atmospheric Pollutants Program with OH radical in vapor phase (Meylan & Howard 1993)

$k_{OH}(\text{calc}) = 0.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 2.74 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: biodegradation rate constant $k = 0.029\text{--}0.042 \text{ h}^{-1}$ in 30 mg L^{-1} activated sludge after a time lag of 15–20 h (Urano & Kato 1986b);

rate constants: $k = 0.022 \text{ d}^{-1}$ in ground water, $k = 0.083 \text{ d}^{-1}$ in river waters and $k = 0.155 \text{ d}^{-1}$ in Superior harbor waters (Vaishnav & Babeu 1987).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated photooxidation $t_{1/2} \sim 22$ d in atmosphere, based on the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson 1988; quoted, Howard 1993); atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: biodegradation $t_{1/2} = 8$ d in river water and $t_{1/2} = 4.5$ d in lake water (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993) and $t_{1/2} = 4$ d in Superior harbor waters (Vaishnav & Babeu 1987).

Ground water: biodegradation $t_{1/2} = 32$ d (Vaishnav & Babeu 1986, 1987; quoted, Howard 1993); estimated $t_{1/2} \sim 0.01$ yr at Noordwijk (Zoeteman et al. 1981).

Sediment:

Soil:

Biota:

TABLE 12.1.2.9.1
Reported aqueous solubilities and Henry’s law constants of acetophenone at various temperatures

Aqueous solubility		Henry’s law constant			
Stephenson 1992		Betterton 1991		Allen et al. 1998	
shake flask-GC/TC		gas stripping-GC		EPICS-UV	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
19.9	5620	14.9	0.582	15	0.263
29.5	7100	25.1	0.921	17.5	0.362
39.5	8330	35.0	2.068	20	0.463
49.8	8140	45.0	4.053	25	1.065
60.1	8880	$\Delta H/(\text{kJ mol}^{-1}) = -50.5$		$\ln K_{\text{AW}} = A - B/(T/\text{K})$ eq. 1 K_{AW} A -9100 B 22.47 $\Delta H/(\text{kJ mol}^{-1}) = -75.6$ $\Delta S/(\text{J K}^{-1} \text{mol}^{-1}) = 186.9$	
70.2	9920				
80.1	12040				

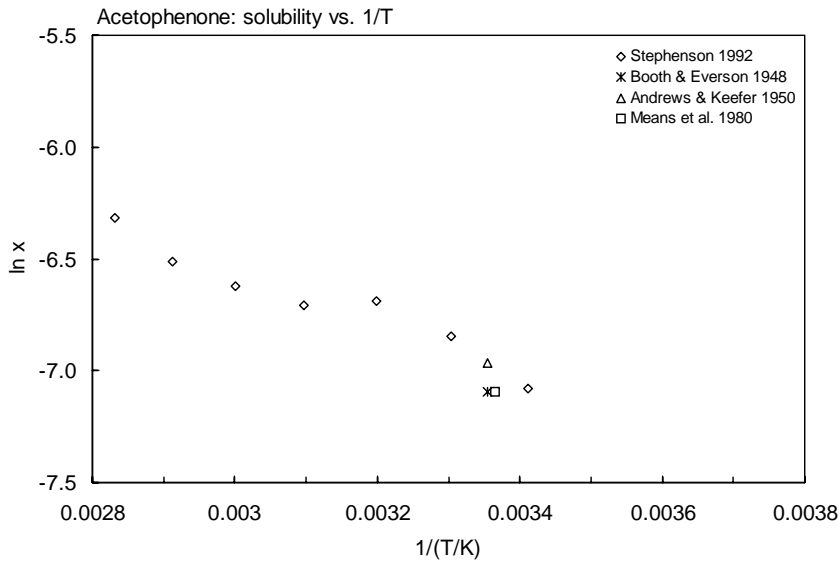


FIGURE 12.1.2.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for acetophenone.

TABLE 12.1.2.9.2

Reported vapor pressures of acetophenone at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Kahlbaum 1898		Stull 1947	
static method-manometer*		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
50.2	266.6	37.1	133.3
56.0	400.0	64.0	666.6
61.0	533.3	78.0	1333
65.0	666.6	92.4	2666
79.0	1333.2	109.4	5333
87.3	1999.8	119.8	7999
93.4	2666.4	133.6	13332
102.4	3999.7	154.2	26664
109.7	5332.9	178.0	53329
114.7	6666.1	202.4	101325
125.2	9999.2		
133.2	13332	mp/°C	20.5
154.1	26664		
167.6	39997		
177.7	53329		
185.7	66661		
192.5	79993		
198.5	93326		
201.5	101325		

*complete list see [ref.](#)

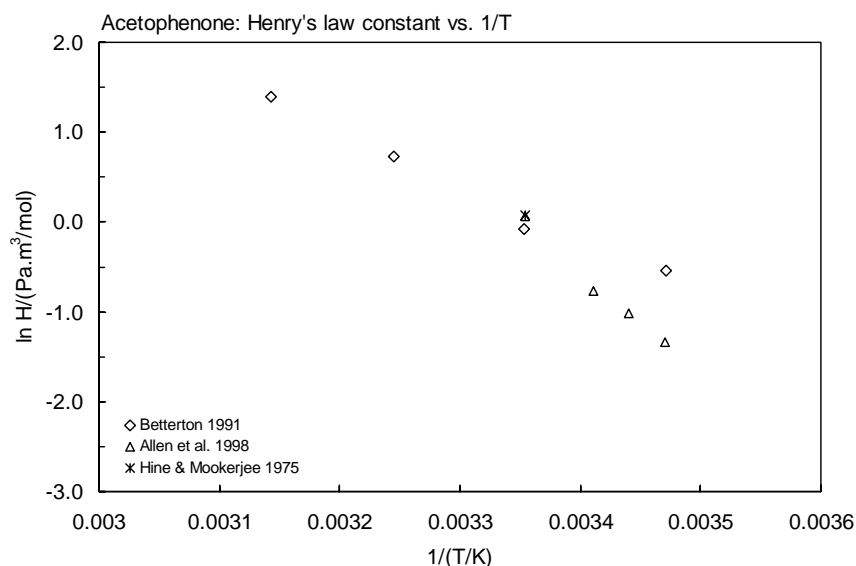


FIGURE 12.1.2.9.2 Logarithm of Henry's law constant versus reciprocal temperature for acetophenone.

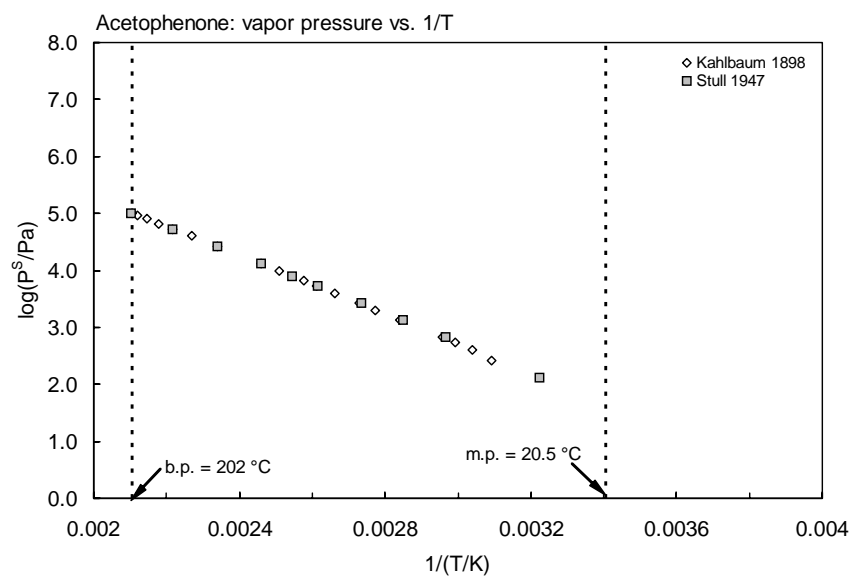
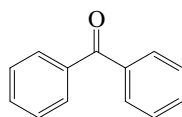


FIGURE 12.1.2.9.3 Logarithm of vapor pressure versus reciprocal temperature for acetophenone.

12.1.2.10 Benzophenone



Common Name: Benzophenone

Synonym: diphenyl ketone, diphenyl methanone

Chemical Name: benzophenone, diphenyl ketone

CAS Registry No: 119-61-9

Molecular Formula: $C_{13}H_{10}O$, $C_6H_5COC_6H_5$

Molecular Weight: 182.217

Melting Point ($^{\circ}C$):

48.1 (α , Weast 1982–83; Dean 1985)

26.0 (β , Weast 1982–83; Dean 1985)

47.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

305.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.6077 (α , $19^{\circ}C$, Weast 1982–83)

1.6059 (β , $23^{\circ}C$, Weast 1982–83)

1.111 ($18^{\circ}C$, Lide 2003)

Molar Volume (cm^3/mol):

206.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

Enthalpy of Vaporization, ΔH_v (kJ/mol):

53.38, 81.90 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

16.99 (Dreisbach 1955)

13.36 (Yalkowsky & Valvani 1980)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.596 (mp at $47.9^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

20720, 21000 (calculated- ΔS_{fus} and mp, estimated, Yalkowsky & Valvani 1980)

276 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

77.7 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

33330* ($257.15^{\circ}C$, temp range 257.15 – $302.85^{\circ}C$, Jaquerod & Wassher 1904; quoted, Boublik et al. 1984)

0.617* (extrapolated-regression tabulated data, temp range 108.3 – $305.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.81086 - 2643.0/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

6287* ($200.50^{\circ}C$, ebulliometry, measured range 200.50 – $306.1^{\circ}C$, Dreisbach & Shrader 1949)

1.242 (calculated by formula, Dreisbach 1955)

$\log(P/mmHg) = 7.28937 - 2144.6/(181.0 + t/^{\circ}C)$; temp range 1980 – $600^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log(P/mmHg) = [-0.2185 \times 14725.4/(T/K)] + 8.456678$; temp range 108.2 – $305.4^{\circ}C$ (Antoine eq., Weast 1972–73)

3.146* ($55.9^{\circ}C$, effusion method, measured range 55.9 – $71.2^{\circ}C$, DePablo 1976)

0.086, 0.0115 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.2931 - 2056.386/(173.545 + t/^{\circ}C)$, temp range 200.5 – $306.1^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.37814 - 2127.915/(181.209 + t/^{\circ}C)$, temp range 257.1 – $302.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.080 (extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.34966 - 2331.4/(195.0 + t/^{\circ}\text{C})$, temp range 48–202°C (Antoine eq., Dean 1985, 1992)

$\log (P/\text{mmHg}) = 7.16294 - 2051.855/(173.074 + t/^{\circ}\text{C})$; temp range 200–306°C (Antoine eq., Dean 1985, 1992)

0.086, 0.095 (interpolated-eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 12.44989 - 4924.329/(T/\text{K})$; temp range 293–318 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 11.736 - 4698/(T/\text{K})$; temp range 298–318 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.41427 - 2144.6/(-92.15 + T/\text{K})$; temp range 433–673 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 16.4144 - 3.8064 \times 10^3/(T/\text{K}) - 2.3984 \cdot \log (T/\text{K}) - 7.4544 \times 10^{-4} \cdot (T/\text{K}) + 2.9345 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 321–816 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.18 (shake flask-UV, Leo et al. 1971)

3.58 (shake flask-UV, Holmes & Lough 1976)

3.10 (shake flask-UV, Unger & Chiang 1981)

3.02 (HPLC- k' correlation, McDuffie 1981)

3.03 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)

3.18 (recommended, Sangster 1989, 1993)

3.18 (recommended, Hansch et al. 1995)

3.09 (microemulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

3.32 (RP-HPLC-RT correlation using short ODP column, Donovan & Pescatore 2002)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

2.63 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 12.1.2.10.1

Reported vapor pressures of benzophenone at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Jaquerod & Wassher 1904		Stull 1947		Dreisbach & Shrader 1949		DePablo 1976	
in Boublik et al. 1984#		summary of lit. data		ebulliometry		effusion method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
257.15	33330	108.2	133.3	200.50	6287	55.9	3.146
260.05	35997	141.7	666.6	206.42	7605	60.7	4.280
265.56	41330	157.6	1333	211.76	8851	66.9	7.146
270.65	46663	175.8	2666	215.46	10114	71.2	9.533
275.23	51996	195.7	5333	231.57	16500		
280.40	58662	208.2	7999	266.87	42066		
285.11	65328	224.4	13332	287.23	67661		
290.26	73327	249.8	26664	306.1	101325		
295.00	81326	276.8	53329				
300.11	91992	305.4	101325				
302.85	95992						
complete data set see ref.		mp/°C	48.5	Antoine eq. given by Dreisbach & Martin 1949			
eq. in Boublik et al. 1984				Eq. 2	P/mmHg		
eq. 2				A	7.81086		
A				B	2643.0		
B				C	230		
C				bp/°C	306.10		
bp/°C				mp/°C	47.93		

Jaquerod, A. Wassher, E. Ber. 3, 2531 (1904)

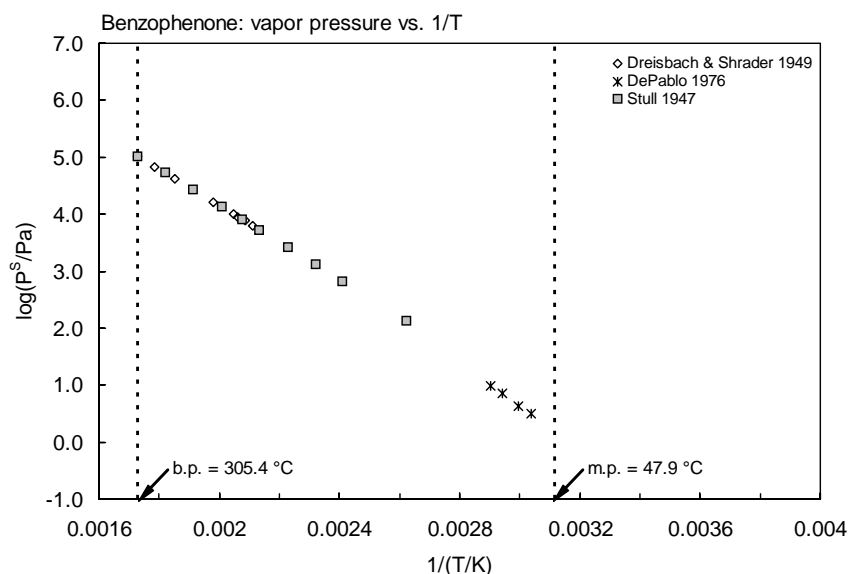


FIGURE 12.1.2.10.1 Logarithm of vapor pressure versus reciprocal temperature for benzophenone.

12.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 12.2.1

Summary of physical properties of aldehydes and ketones

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol	
							MW/ρ at 20°C	Le Bas cm ³ /mol
Aldehydes:								
Methanal (Formaldehyde)	50-00-0	HCHO	30.026	−92	−19.1	1		29.6
Ethanal (Acetaldehyde)	75-07-0	CH ₃ CHO	44.052	−123.37	20.1	1	56.23#	51.8
Propanal (Propionaldehyde)	123-38-6	C ₂ H ₅ CHO	58.079	−80	48	1	72.87	74.0
Butanal (<i>n</i> -Butyraldehyde)	123-72-8	C ₃ H ₇ CHO	72.106	−96.86	74.8	1	89.95	96.2
Isobutraldehyde	78-84-2	<i>i</i> C ₃ H ₇ CHO	72.106	−65.9	64.5	1	91.38	96.2
Pentanal (<i>n</i> -Valeraldehyde)	110-62-3	C ₄ H ₉ CHO	86.132	−91.5	103	1	106.40	118.4
Hexanal	66-25-1	C ₅ H ₁₁ CHO	100.158	−56	131	1	120.17	140.6
Heptanal	111-71-7	C ₆ H ₁₃ CHO	114.185	−43.4	152.8	1	140.41**	162.8
Octanal	124-13-0	C ₇ H ₁₅ CHO	128.212		171	1	156.15	185.0
2-Propenal (Acrolein)	107-02-8	H ₂ C=CHCHO	56.063	−87.7	52.6	1	66.83	66.6
2-Butenal	123-73-9	CH ₃ CH=CHCHO	70.090	−76	102.2	1	82.30	88.8
Furfural (2-Furaldehyde)	98-01-1	C ₅ H ₄ O ₂	96.085	−38.1	161.7	1	82.83	92.1
Benzaldehyde	100-52-7	C ₆ H ₅ CHO	106.122	−57.1	178.8	1	101.59	118.2
Ketones:								
Acetone	67-64-1	CH ₃ COCH ₃	58.079	−94.7	56.05	1	73.53	74.0
2-Butanone (Methyl ethyl ketone)	78-93-3	C ₂ H ₅ COCH ₃	72.106	−86.64	79.59	1	89.53	96.2
2-Pentanone	107-87-9	C ₃ H ₇ COCH ₃	86.132	−76.8	102.26	1	106.81	118.4
3-Pentanone	96-22-0	CH ₃ CH ₂ COCH ₂ CH ₃	86.132	−39	101.7	1	105.77	118.4
Methyl isobutyl ketone (MIBK)	108-10-1	(CH ₃) ₂ CHCH ₂ COCH ₃	100.158	−84	116.5	1	125.04	140.6
2-Hexanone	591-78-6	C ₄ H ₉ COCH ₃	100.158	−55	127.6	1	123.45	140.6
2-Heptanone	110-43-0	CH ₃ (CH ₂) ₄ COCH ₃	114.185	−35	151.05	1	140.04	162.8
2-Octanone	111-13-7	C ₇ H ₁₆ CO	128.212	−16	172.5	1	156.36	185.0
Cyclopentanone	120-92-3	C ₄ H ₈ CO	84.117	−51.90	130.57	1	88.67	99.5
Cyclohexanone	108-94-1	C ₅ H ₁₀ CO	98.142	−27.9	155.43	1	103.83	118.2
Acetophenone	98-86-2	C ₆ H ₅ COCH ₃	120.149	20.5	202	1	116.87	140.4
Benzophenone	119-61-9	C ₆ H ₅ COC ₆ H ₅	182.217	47.9	305.4	0.596	164.01#	206.8

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$; # at 18°C; ** at 25°C.

TABLE 12.2.2
Summary of selected physical-chemical properties of aldehydes and ketones at 25°C

Compound	Selected properties					Henry's law constant H/(Pa·m³/mol)				
	Solubility		Vapor pressure		log K _{OW}	calcd P/C	exptl (a)	exptl (b)	exptl (c)	exptl (c)
	S/(g/m³)	C _L /(mol/m³)	P _S /Pa	P _L /Pa						
Aldehydes:										
Methanal	miscible	miscible	517000	517000	0.35			0.0298		0.0341
Ethanal	miscible	miscible	121300	121300	0.45		6.69	6.80	8.00	8.90
Propanal	310000	5338	42400	42400	0.59	7.944	7.44	8.40	7.51	
Butanal	71000	984.7	15200	15200	0.88	15.44	11.65	11.65		
<i>n</i> -Valeraldehyde			2180	2180			14.87	15.59		
Hexanal	5020	50.12			1.78		21.57	19.49		
2-Propenal (Aroclein)	208000	3710	36500	36500	−0.10	9.838	13.37		13.17	
2-Butenal	15600	222.6	5100	5100		22.91				
Furfural	79400	826.4	310	310	0.41	0.3751				
Benzyldehyde	3000	28.27	174	174	1.48	6.155	2.28			2.71
Ketones:										
Acetone	miscible	miscible	30806	30800	−0.24		3.97		3.93	3.07
2-Butanone	240000	3328.4	12100	12100	0.29	3.635	9.71		5.76	
2-Pentanone	59500	690.8	4720	4720	0.84	6.833	6.44			
3-Pentanone	34000	394.7	4700	4700	0.82	11.91				
Methyl isobutyl ketone	17000	169.7	2600	2600		15.32				
2-Hexanone	17500	174.7	1600	1600	1.38	9.157				
2-Heptanone	4300	37.66	500	500	2.08	13.28	14.73			
2-Octanone	1130	8.814	180	180	2.37	20.42	19.09			
Cyclopentanone			1540	1540						
Cyclohexanone	23000	234.4	620	620	0.81	2.646				
Acetophenone	5500	45.78	45	45	1.63	0.983				0.92
Benzophenone	276	2.541	0.09	0.151	3.18	0.059				

(a) Butler et al. 1935; Buttery et al. 1969; (b) Zhou & Mopper 1990; (c) Snider & Dawson 1985; (d) Betterton & Hoffmann 1988.

TABLE 12.2.3

Suggested half-life classes for aldehydes and ketones at various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aldehydes:				
Methanal (Formaldehyde)	1	3	3	4
Ethanal (Acetaldehyde)	1	3	3	4
Propanal (Propionaldehyde)	1	3	3	4
Butanal (<i>n</i> -Butyraldehyde)	1	3	3	4
2-Propenal (Acrolein)	1	3	3	4
2-Butenal	1	3	3	4
Furfural (2-Furaldehyde)	1	3	3	4
Benzaldehyde	1	3	3	4
Ketones:				
Acetone	4	3	4	5
2-Butanone (Methyl ethyl ketone)	4	3	3	5
2-Pentanone	3	4	4	5
3-Pentanone	3	4	4	5
Methyl isobutyl ketone (MIBK)	3	4	4	5
2-Hexanone	3	4	4	5
2-Heptanone	3	4	4	5
Cyclohexanone	3	4	4	5
Acetophenone	5	4	4	5
Benzophenone	5	4	4	5

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

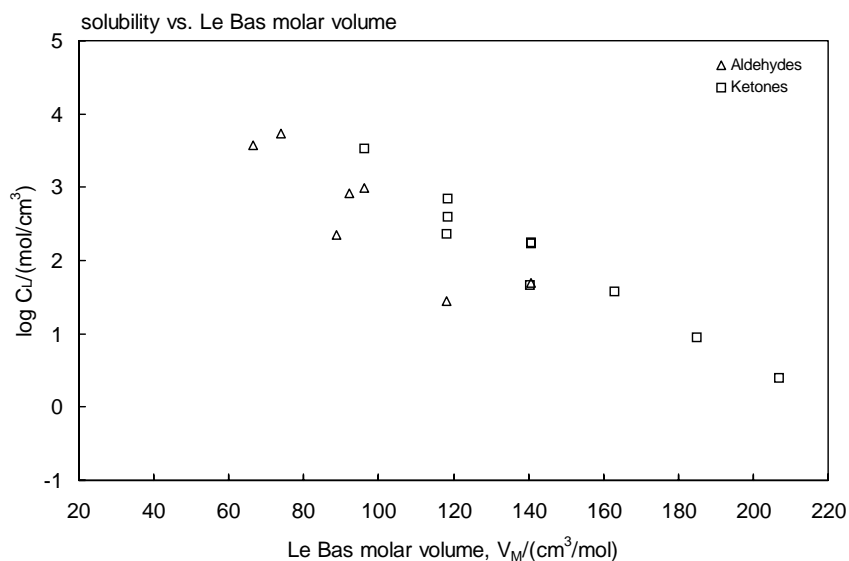


FIGURE 12.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.

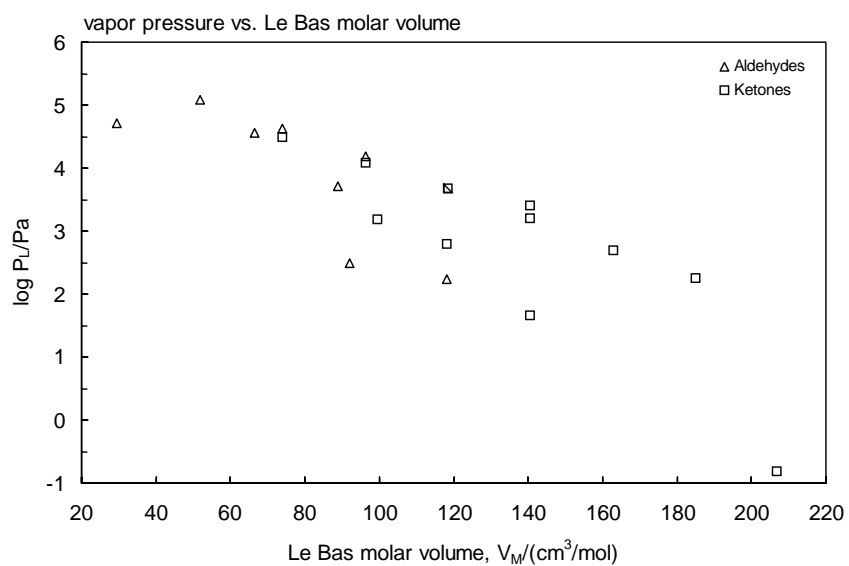


FIGURE 12.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for aldehydes and ketones.

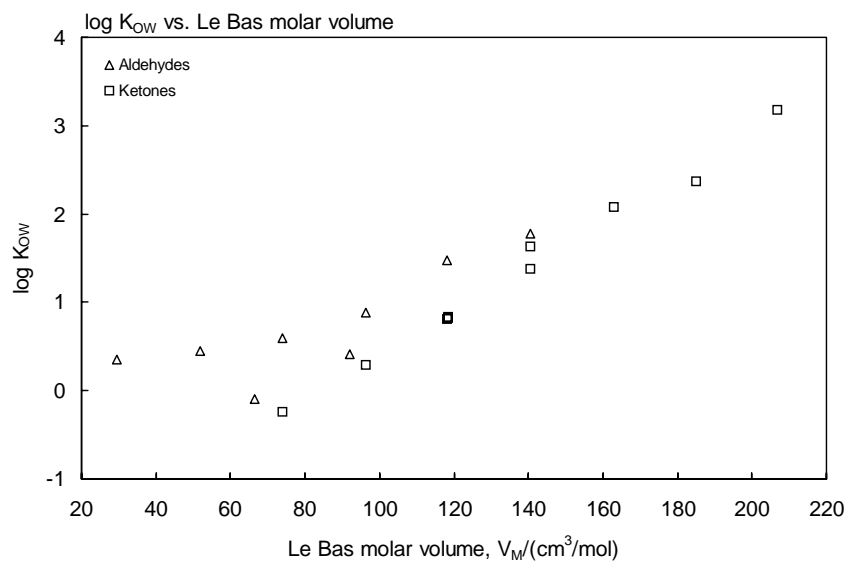


FIGURE 12.2.3 Octanol-water partition coefficient versus Le Bas molar volume for aldehydes and ketones.

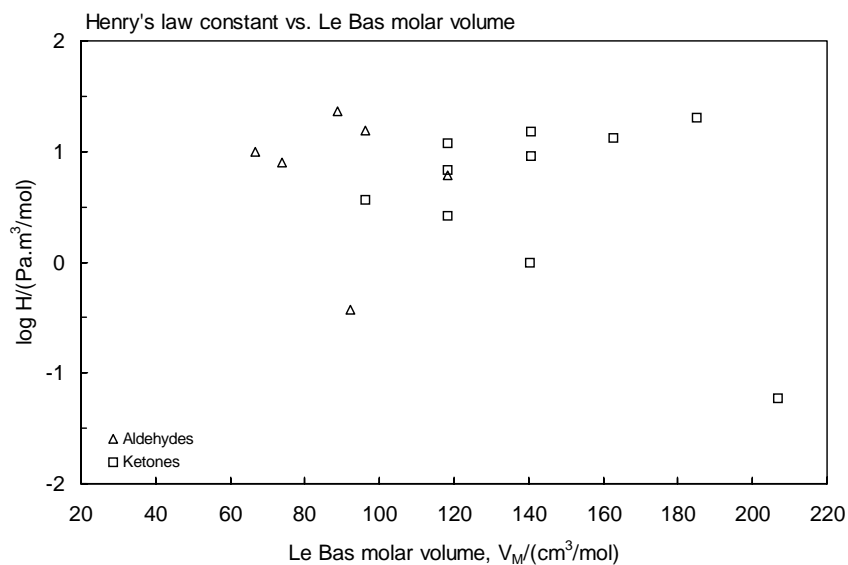


FIGURE 12.2.4 Henry's law constant versus Le Bas molar volume for aldehydes and ketones.

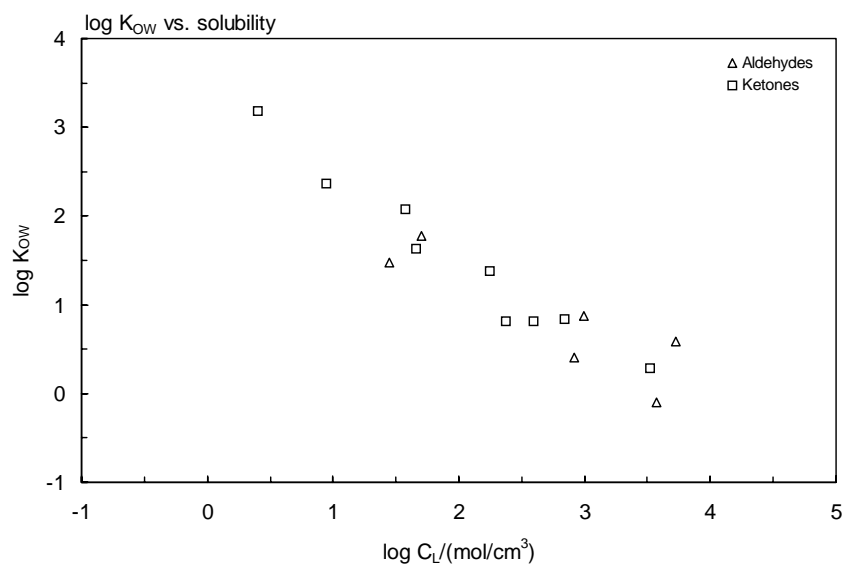


FIGURE 12.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for aldehydes and ketones.

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13 Carboxylic Acids

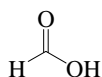
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13.1 LIST OF CHEMICALS AND DATA COMPILATIONS

13.1.1 ALIPHATIC ACIDS

13.1.1.1 Formic acid



Common Name: Formic acid

Synonym: methanoic acid

Chemical Name: formic acid

CAS Registry No: 64-18-6

Molecular Formula: CH₂O₂, HCOOH

Molecular Weight: 46.026

Melting Point (°C):

8.3 (Lide 2003)

Boiling Point (°C):

101 (Lide 2003)

Density (g/cm³ at 20°C):

1.21961, 1.21328 (20°C, 25°C, Dreisbach & Martin 1949)

1.2200 (Weast 1982–83; Dean 1985)

1.2141 (25°C, Riddick et al. 1986)

Molar Volume (cm³/mol):

37.7 (calculated-density, Stephenson & Malanowski 1987)

46.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:3.751 (pK_a, Dean 1985)3.752 (pK_a, Riddick et al. 1986)3.740 (pK_a, Sangster 1989)

3.800 (Kollig 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.68 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):Fugacity Ratio at 25°C (assuming ΔS_{fus} = 13.5 J/mol K), F: 1.0Water Solubility (g/m³ or mg/L at 25°C):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4344* (24.6°C, temp range 21.8–100.6°C, Kahlbaum 1894)

5333* (24°C, compiled and evaluated data, temp range –20 to 100.6°C, Stull 1947)

log (P/mmHg) = 7.15689 – 1414.1/(230 + t/°C) (Antoine eq., Dreisbach & Martin 1949)

10114* (37.75°C, ebulliometry, measured range 37.75–100.7°C, Dreisbach & Shrader 1949)

log (P/mmHg) = [–0.2185 × 9896.5/(T/K)] + 8.779337; temp range –20 to 100.6°C (Antoine eq., Weast 1972–73)

4666, 7198 (20°C, 30°C, Verschuereen 1983)

5720, 5744, 4420 (calculated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 4.09278 – 539.775/(136.826 + t/°C); temp range 0.5–34.2°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 6.69157 – 1689.096/(259.726 + t/°C); temp range 37.35–100.7°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)

log (P/kPa) = 3.7279 – 295.021/(70.7 + t/°C); temp range 21–100.6°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- 5744 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.5818 - 1699.2/(260.7 + t/^{\circ}\text{C})$; temp range: 37–101°C (Antoine eq., Dean 1985, 1992)
 5750 (selected, Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.50280 - 1563.28/(247.06 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 5733* (comparative ebulliometry, measured range 299.8–393 K, Ambrose & Ghassee 1987)
 $\ln (P/\text{kPa}) = 15.40560 - 3894.764/[(T/\text{K}) - 13.0]$; temp range 299.8–393 K (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghassee 1987)
 5711 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.611 - 3160/(T/\text{K})$; temp range 268–281 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.5028 - 1563.28/(-26.09 + T/\text{K})$; temp range 283–384 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
 5680, 67850 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 27.9278 - 2.5976 \times 10^3/(T/\text{K}) - 7.2489 \cdot \log (T/\text{K}) + 6.411 \times 10^{-10} \cdot (T/\text{K}) + 3.9421 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 282–580 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

- 0.0181 (calculated, Keene & Galloway 1986)
 0.0274 (calculated, Jacob 1986)
 0.017 (pH 4, Gaffney et al. 1987)
 0.112 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
 0.0076, 0.0098, 0.0178 (24°C, bubble column technique, concn: of 1, 10, 10⁵ ppm, Servant et al. 1991)
 0.0281 (Betterton 1992)
 0.018 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)
 $\ln [k_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -10.31 + 5634/(T/\text{K})$, temp range 178.15–308.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0183 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
 0.018–0.028 (calculated-thermodynamic data, Johnson et al. 1996)
 0.0118, 0.00921 (counter-flow packed column technique-ion chromatography; "best" exptl. value, Johnson et al. 1996)
 $\ln [k_H/(\text{M/atm})] = -11.04 + 6100/(T/\text{K})$; temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)
 0.0137 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 1996)
 0.0107 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 2.914 - 2425/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- −0.54 (shake flask-titration, Collander 1951; quoted, Leo et al. 1971; Hansch et al. 1972; Hansch & Leo 1979)
 −0.54 (shake flask-titration, Whitehead & Geankoplis 1955)
 −0.46 (calculated-f const., Rekker & de Kort 1979)
 −0.54 (recommended, Sangster 1989)
 −0.54 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

- −0.27 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or the Arrhenius expression see reference:

$k_{\text{OH}} = (3.2 \pm 1.0) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982)

$k = (100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ at pH 8; $(5 \pm 5) \text{ M}^{-1} \text{ s}^{-1}$ for protonated species; $(100 \pm 20) \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water using 1 mM propyl alcohol as scavenger at pH 2.0–4.0 and 20–23°C (Hoigné & Bader 1983b)

$k_{\text{OH}}^* = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–430 K (flash photolysis-resonance fluorescence, Wine et al. 1985)

$k_{\text{OH}} = (2.95 \pm 0.07) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance absorption, Jolly et al. 1986)

$k_{\text{OH}} = (3.7 \pm 0.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-RF, Dagaut et al. 1988)

$k_{\text{OH}}^* = (2.69 \pm 0.17) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $4.47 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 297 K, measured range 297–445 K (laser photolysis-resonance absorption, Singleton et al. 1988)

$k_{\text{OH}} = 3.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k(\text{soln}) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with hydroxyl radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}}^* = 4.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 7.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.1.1.1

Reported vapor pressures of formic acid at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3) \quad \ln (P/\text{Pa}) = A - B/(C + T/K) \quad (3a)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Kahlbaum 1894		Stull 1947		Dreisbach & Shrader 1949		Ambrose & Ghiassie 1987	
Ber. 16, 2476		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
21.8	3312	−20.0	133	37.75	10114	299.789	6188
22.6	3688	−5.0	666.6	48.79	16500	302.006	6876
24.6	4344	2.10	1333	73.55	42066	307.578	8881
27.9	5520	10.3	2666	87.82	67661	308.389	9230
30.5	6621	24.0	5333	100.7	101325	310.035	9896
37.8	9938	32.4	7999			313.764	11668
100.6	101325	43.8	13332	bp/°C	100.7	316.803	13293
		61.4	26664			319.729	15031
		80.3	53329			324.842	18432
		100.6	101325			326.895	20105
						329.030	21830
		mp/°C	8.2			332.807	25236
						336.159	28640
						342.086	35456
						344.582	38845
						346.997	43226
						349.134	45630

TABLE 13.1.1.1.1 (Continued)

Kahlbaum 1894		Stull 1947		Dreisbach & shrader 1949		Ambrose & Ghiassee 1987	
Ber. 16, 2476		summary of literature data		ebulliometry		comparative ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
						350.313	47321
						353.362	52449
						355.215	55868
						↓	↓
						392.654	172035
						298.15	5733
						Antoine eq.	
						eq. 3a	P/kPa
						A	15.40560
						B	3894.764
						C	−13.0
						bp/K	374.04

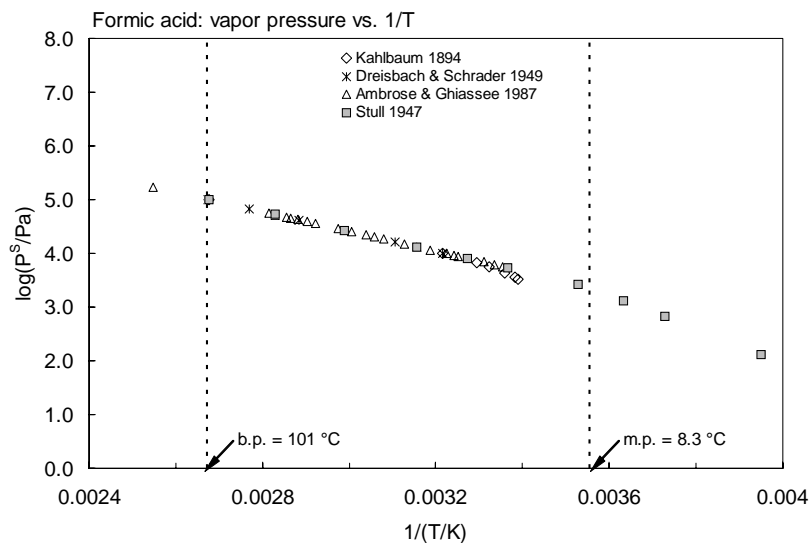


FIGURE 13.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for formic acid.

13.1.1.2 Acetic acid



Common Name: Acetic acid

Synonym: ethanoic acid, methanecarboxylic acid, glacial acetic, vinegar acid

Chemical Name: acetic acid

CAS Registry No: 64-19-7

Molecular Formula: CH_3COOH

Molecular Weight: 60.052

Melting Point ($^{\circ}\text{C}$):

16.64 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

117.9 (Weast 1982–83; Dean 1985; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at 20°C):

1.04923, 1.04365 (20°C , 25°C , Dreisbach & Martin 1949)

1.0492 (Weast 1982–83; Dean 1985)

Molar Volume (cm^3/mol):

57.1 (calculated-density, Rohrschneider 1973)

68.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.733 (pK_a , Korman & La Mer 1936)

4.760 (pK_a , Fieser & Fieser 1958; Sangster 1989)

4.750 (pK_a , Weast 1982–83; Howard 1990)

4.756 (pK_a , Dean 1985; Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.72 (Ambrose et al. 1977; Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

miscible (Dean 1985; Riddick et al. 1986)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2040* (interpolated-regression of tabulated data, temp range -17.2 – 118°C , Stull 1947)

$\log (\text{P}/\text{mmHg}) = 7.45144 - 1589.3/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

10114* (55.75°C , ebulliometry, measured range 55.75 – 117.72°C , Dreisbach & Shrader 1949)

2666* (29.8°C , static method-manometer, measured range 29.8 – 126.45°C , Potter & Ritter 1954)

8297* (52.36°C , ebulliometry, measured range 52.36 – 118.14°C , McDonald et al. 1959)

$\log (\text{P}/\text{mmHg}) = 7.55716 - 1642.54/(233.386\text{C} + t/^{\circ}\text{C})$; temp range 52 – 118°C (ebulliometry, McDonald et al. 1959)

2105 (calculated by formula, Dreisbach 1961)

$\log (\text{P}/\text{mmHg}) = 7.18807 - 1416.7/(211 + t/^{\circ}\text{C})$, temp range 36 – 170°C , (Antoine eq. for liquid state, Dreisbach 1961)

2030 (Hoy 1970)

$\log (\text{P}/\text{mmHg}) = [-0.2185 \times 9963.9/(T/\text{K})] + 8.50200$; temp range -35 to 10°C (Antoine eq., Weast 1972–73)

$\log (\text{P}/\text{mmHg}) = [-0.2185 \times 9486.6/(T/\text{K})] + 8.142405$; temp range -17.2 to 312.5°C (Antoine eq., Weast 1972–73)

2079* (ebulliometry, fitted to Antoine eq., measured range 304.065 – 415.041 K , Ambrose et al. 1977)

$\log (\text{P}/\text{kPa}) = 6.66686 - 1633.288/[(T/\text{K}) - 40.626]$; temp range 351.347 – 415.041 K (Antoine eq.-I, ebulliometry, Ambrose et al. 1977)

- $\log (P/\text{kPa}) = 6.59795 - 1587.182/\{(T/\text{K}) - 45.392\}$; temp range 304.065–415.041 K (Antoine eq.-II, ebulliometry, Ambrose et al. 1977)
 1520, 2666 (20°C, 30°C, Verschuereen 1983)
 2088 (extrapolated average-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.5039 - 1527.764/(221.742 + t/^{\circ}\text{C})$, temp range 29.8–126.45°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.72515 - 1670.427/(236.091 + t/^{\circ}\text{C})$, temp range 52.36–118.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 2050 (calculated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.38782 - 1533.313/(222.309 + t/^{\circ}\text{C})$, temp range: liquid (Antoine eq., Dean 1985, 1992)
 2079 (Riddick et al. 1986)
 $\log (P/\text{kPa}) = 6.66686 - 1633.288/(232.885 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 2076 (comparative ebulliometry data, Ambrose & Ghassee 1987)
 $\ln (P/\text{kPa}) = 15.19234 - 3654.622/[(T/\text{K}) - 45.392]$ (Antoine eq. Ambrose & Ghassee 1987)
 2114 (calculated-Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 7.672 - 2177/(T/\text{K})$, temp range: 238–283 K, (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 9.9268 - 2847/(T/\text{K})$; temp range 243–289 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.68206 - 1642.54/(-39.764 + T/\text{K})$; temp range 289–392 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.39226 - 2258.22/(2762 + T/\text{K})$; temp range 391–550 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.5729 - 1572.32/(-46.777 + T/\text{K})$; temp range 290–396 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.82561 - 1748.572/(-28.259 + T/\text{K})$; temp range 391–447 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 7.22638 - 2010.805/(12.244 + T/\text{K})$; temp range 437–535 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.44129 - 3628.409/(182.674 + T/\text{K})$; temp range 525–593 K (Antoine eq.-VIII, Stephenson & Malanowski 1987)
 1520, 32660 (measured, calculated-solvatochromic parameters., Banerjee et al. 1990)
 $\log (P/\text{mmHg}) = 28.3756 - 2.9734 \times 10^3/(T/\text{K}) - 7.032 \cdot \log (T/\text{K}) - 1.5051 \times 10^{-9} \cdot (T/\text{K}) + 2.1806 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 290–593 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$) at 25°C and reported temperature dependence equations):

- 0.0303 (partial pressure, Butler & Ramchandani 1935)
 0.0305 (exptl., Hine & Mookerjee 1975)
 0.0300, 0.0280 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.0115 (calculated, Keene & Galloway 1986)
 0.0101 (effective Henry's law constant, pH 4, Gaffney et al. 1987)
 0.0254 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.121 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)
 0.0101, 1.01×10^{-4} (at pH 4, pH 7, Howard 1990)
 0.0109, 0.00905, 0.0158 (23°C, bubble column technique, concn: 1, 10, 10^5 ppm. Servant et al. 1991)
 0.0184 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)
 $\ln [K_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -25.67 + 8322/(T/\text{K})$, temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0285 (calculated-bond contribution, Brimblecombe et al. 1992)
 0.0431 (calculated-molecular structure, Russell et al. 1992)
 0.0182 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)
 0.0115–0.0195 (calculated-thermodynamic data, Johnson et al. 1996)
 0.0245, 0.0145 (counter-flow packed column technique-ion chromatography; "best" exptl value, Johnson et al. 1996)

$\ln [K_H/(M/atm)] = -12.5 + 6200/(T/K)$, temp range 2–35°C (counter-flow packed column measurements, Johnson et al. 1996)

0.0130 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.0154 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.650 - 2596/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

-0.30 (shake flask-titration, Leonard et al. 1948)

-0.31 (shake flask-titration, Collander 1951)

-0.29; -0.17 (calculated-fragment const.; calculated- π const., Rekker 1977)

-0.29 (shake flask-radiochemical method, pH 1, Wolfenden 1978)

-0.17, -0.31 (Hansch & Leo 1979)

-0.17 (shake flask, Log P Database, Hansch & Leo 1987)

-0.17 (recommended, Sangster 1989, 1993)

-0.17 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

4.31 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

< 0.0 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

no detectable sorption (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)

0.00 (soil, quoted exptl., Meylan et al. 1992)

-0.21 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

0.00 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (0.6 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 26.7 \text{ d}$ for the vapor-phase reaction with 5×10^5 hydroxyl radical/ cm^3 in air at 25°C (flash photolysis-resonance fluorescence technique, Zetzsch & Stuhl 1982; quoted, Atkinson 1985)

$k(\text{aq.}) \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water; $k \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k \leq 3 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2.0–5.5 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH}^* = (7.4 \pm 0.6) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-resonance fluorescence, Dagaut et al. 1988)

$k_{OH} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air, and $k(\text{soln}) = 2.70 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH} = 7.4 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1990)

$k_{OH}(\text{calc}) = 0.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996).

Hydrolysis:

Biodegradation: > 90% degradation in 3 d using an activated sludge inoculum; in 24 h in batch aeration in sewage and 14 d using sediment from the Rhine river as inocula (Howard 1990).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 26.7 \text{ d}$, based on measured rate constant of $0.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with 5×10^5 hydroxyl radicals/ cm^3 in air at 25°C (Atkinson 1985; quoted, Howard 1990).

Surface water: $t_{1/2} = 26\text{--}46 \text{ yr}$, based on OH radical concn. in sunlit natural water of $1 \times 10^{-17} \text{ mol/L}$ (Howard 1990).

Groundwater:

Sediment: > 90% degradation in 14 d using Rhine River sediment as inocula (Kool 1984; quoted, Howard 1990).

Soil:

Biota:

TABLE 13.1.1.2.1

Reported vapor pressures of acetic acid at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Dreisbach & Shrader 1949		Potter & Ritter 1954		McDonald et al. 1959	
summary of literature data		ebulliometry		static method-manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
−17.2	133	55.75	10114	29.8	2666	52.36	8297
6.3	666.6	66.07	16500	40.25	4693	55.63	9998
17.5	1333	91.13	42066	51.08	8013	67.20	16517
29.9	2666	117.72	101325	55.54	9866	91.49	42302
43	5333			60.93	12599	105.49	68210
51.7	7999	bp/°C	100.79	65.50	15332	115.51	94156
63	13332			71.04	19345	116.83	98175
80	26664			75.70	23105	117.27	99584
99	53329			80.41	28038	117.71	110901
118.1	101325			85.69	34224	118.14	102318
				90.59	40930		
mp/°C	16.7			95.66	48982	eq. 2	P/mmHg
				100.29	57488	A	7.55716
				105.45	68314	B	1642.54
				110.0	79193	C	233.386
				115.12	92992		
				118.41	102978	mp/°C	16.34
				122.44	116137		
				123.86	121256		
				126.45	130669		
				Antoine eq.			
				eq. 2	P/mmHg		
				A	7.4275		
				B	1558.03		
				C	224.79		

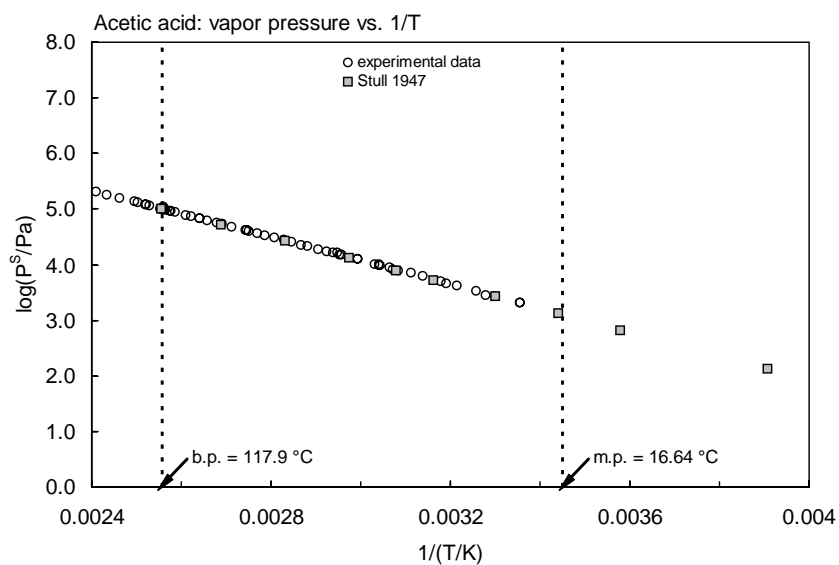
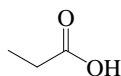


FIGURE 13.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for acetic acid.

13.1.1.3 Propionic acid



Common Name: Propionic acid

Synonym: methylacetic acid, propanoic acid

Chemical Name: propanoic acid, propionic acid

CAS Registry No: 79-09-4

Molecular Formula: $C_3H_6O_2$, CH_3CH_2COOH

Molecular Weight: 74.079

Melting Point ($^{\circ}C$):

−20.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

141.15 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.99336, 0.98797 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9930 (Weast 1982–83)

Molar Volume (cm^3/mol):

74.6 ($20^{\circ}C$, calculated-density)

90.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

−6.80 (pK value, Perrin 1972)

4.874 (Dean 1985; Riddick et al. 1986)

4.870 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.66 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

550* (interpolated-regression of tabulated data, temp range 4.6 – $141.4^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.92234 - 1869.4/(230 + t/^{\circ}C)$, (Antoine eq., Dreisbach & Martin 1949)

7605* ($72.39^{\circ}C$, ebulliometry, measured range 72.39 – $140.80^{\circ}C$, Dreisbach & Shrader 1949)

446 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.35027 - 1497.775/(194.12 + t/^{\circ}C)$, temp range 60 – $185^{\circ}C$ (Antoine eq., Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 12454.4/(T/K)] + 9.647835$; temp range 4.6 – $238^{\circ}C$ (Antoine eq., Weast 1972–73)

435* (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.64344 - 1594.723/[(T/K) - 70.545]$; temp range 328 – $438\ K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

500, 442 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.84202 - 1736.007/(218.032 + t/^{\circ}C)$, temp range 72.39 – $128.34^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.67457 - 1615.227/(204.788 + t/^{\circ}C)$, temp range 55.11 – $164.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

257 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.403 - 950.2/(130.3 + t/^{\circ}C)$, temp range 56 – $139.5^{\circ}C$ (Antoine eq., Dean 1985, 1992)

451 (Riddick et al. 1986)

$\log(P/kPa) = 6.64334 - 1594.273/(202.605 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

452 (comparative ebulliometry, Ambrose & Ghiassee 1987)

$\ln (P/\text{kPa}) = 15.29686 - 3670.949/[(T/\text{K}) - 70.545]$, (Antoine eq., Ambrose & Ghiassie 1987)

$\log (P_L/\text{kPa}) = 6.60267 - 1577.96/(-79.844 + T/\text{K})$, temp range 343–419 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 9.24101 - 12835.99/(-23.07 + T/\text{K})$, temp range 414–511 K (Antoine eq.-II, Stephenson & Malanowski 1987)

453, 8758 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log (P/\text{mmHg}) = 20.2835 - 3.1165 \times 10^3/(T/\text{K}) - 3.6015 \cdot \log (T/\text{K}) - 1.3892 \times 10^{-3} \cdot (T/\text{K}) + 7.1801 \times 10^{-7} \cdot (T/\text{K})^2$; temp range 252–604 K (vapor pressure eq., Yaws 1994)

14560* (88.37°C, VLE still-manometry, measured range 88.37–140.59°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 18.105654 - 5640.3443/[(t/^\circ\text{C}) + 277.46143]$; temp range 88.37–140.59°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.0445 (partial pressure, Butler & Ramchandani 1935)

0.0450 (exptl., Hine & Mookerjee 1975)

0.0420, 0.0430 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.0298 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

0.0163, 0.00151, 0.0289 (23.1°C, bubble column technique, concn: 1, 10, 10^5 ppm. Servant et al. 1991)

0.0180 (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0431 (calculated-bond contribution, Brimblecombe et al. 1992)

0.0177 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.25 (shake flask-titration, Collander 1951)

0.23, 0.24 (calculated- π const., calculated-fragment const., Rekker 1977)

0.33, 0.25 (Hansch & Leo 1979)

0.27 (shake flask-titration, Umland 1983)

0.33 (recommended, Sangster 1989; 1994)

0.33 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = (1.6 \pm 0.5) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982; quoted, Atkinson 1985)

$k = 2.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water, $k \leq 4.0 \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k = (1 \pm 0.5) \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2–5 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH}^* = (1.22 \pm 0.12) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988)

$k_{OH} = 1.22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air and $k(\text{soln}) = 1.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{OH} = (1.22 - 1.60) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 1.35 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.1.3.1

Reported vapor pressures of propionic acid at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)		ln P = A – B/(T/K)		(1a)	
log P = A – B/(C + t/°C)		(2)		ln P = A – B/(C + t/°C)		(2a)	
log P = A – B/(C + T/K)		(3)		ln P = A – B/(C + T/K)		(3a)	
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Dreisbach & Shrader 1949		Ambrose et al. 1981		Clifford et al. 2004	
summary of literature data		ebulliometry		comparative ebulliometry		VLE still-Hg manometer	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
4.60	133.3	72.39	7605	55.174	2891	88.37	14560
28.0	666.6	76.75	8851	57.414	3274	95.22	19580
39.7	1333	79.68	10114	60.143	3787	105.80	29650
52.0	2666	90.73	16500	63.850	4594	113.59	39730
65.8	5333	114.62	42066	67.094	5417	119.78	49790
74.1	7999	128.34	67661	70.860	6529	125.94	59860
85.8	13332	140.80	101325	74.311	7713	129.50	69920
102.5	26664			78.096	9217	133.65	79990
122.0	53329			81.787	10917	137.18	90070
141.5	101325			85.630	12961	138.82	95100
				89.553	15372	140.59	101210
mp/°C	–22			93.303	18022		
				98.207	22058	Antoine eq.	
				102.401	26085	eq. 3a	P/kPa
				107.174	31400	A	18.105654
				111.847	37437	B	56403343
				116.747	44780	C	277.46143
				122.130	54180		
				126.788	63579	data also fitted to Wagner eq.	
				131.723	74946		
				137.045	89022		
				141.105	101143		
				25.0	451		
				eq. 3	P/kPa		
				A	6.64334		
				B	1594.273		
				C	–70.545		
				data also fitted to Chebyshev and Wagner equations			
				bp/K	436.868		

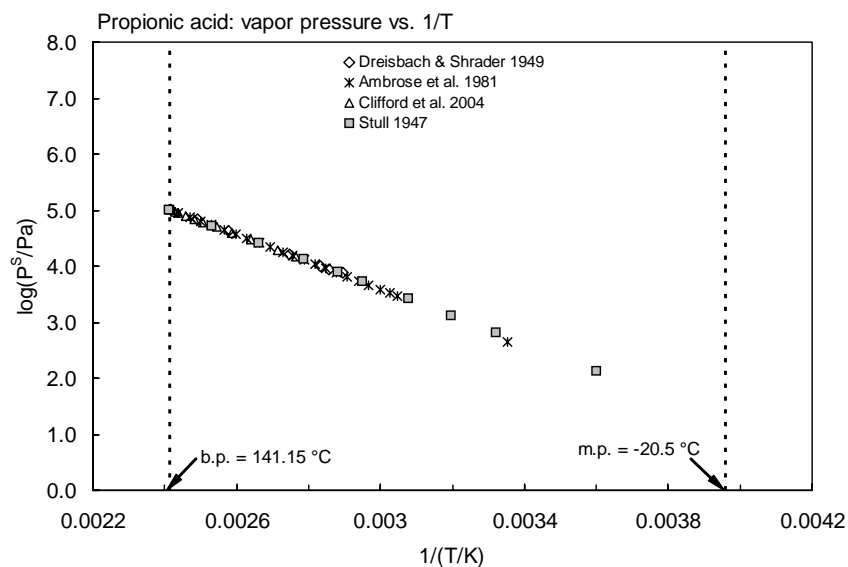
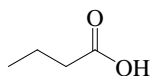


FIGURE 13.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for propionic acid.

13.1.1.4 Butyric acid



Common Name: Butyric acid

Synonym: butanoic acid, *n*-butyric acid, ethylacetic acid

Chemical Name: *n*-butyric acid, butyric acid

CAS Registry No: 107-92-6

Molecular Formula: $C_4H_8O_2$, $CH_3CH_2CH_2COOH$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−5.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

163.75 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.95767, 0.95273 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach & Martin 1949)

0.9582 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.0 ($20^{\circ}C$, calculated-density)

112.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.817 (Dean 1985)

4.822 (Riddick et al. 1986)

4.820 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.6 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($25.5^{\circ}C$, temp range 25.5 – $163.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 8.19524 - 2089.9/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

4716* ($90.92^{\circ}C$, ebulliometry, measured range 90.92 – $163.25^{\circ}C$, Dreisbach & Shrader 1949)

95.77 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.38423 - 1542.6/(179.0 + t/^{\circ}C)$, temp range 82 – $210^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 11881.2/(T/K)] + 8.773450$; temp range 25.5 – $352^{\circ}C$ (Antoine eq., Weast 1972–73)

83.95* (comparative ebulliometry, fitted to Antoine eq., measured range 340 – $452 K$, Ambrose et al. 1981)

$\log(P/kPa) = 6.55643 - 1563.444/[(T/K) - 93.307]$; temp range 339.7 – $452 K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

104, 92 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.8682 - 1766.906/(200.097 + t/^{\circ}C)$, temp range 90.2 – $163.25^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.67596 - 1642.683/(188.013 + t/^{\circ}C)$; temp range 76.53 – $178.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

104.3 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.7399 - 1764.7/(199.9 + t/^{\circ}C)$; temp range 90 – $163^{\circ}C$ (Antoine eq., Dean 1985, 1992)

102.0 (selected, Riddick et al. 1986)

$\log(P/kPa) = 6.55643 - 1563.444/(179.843 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

- 101 (comparative ebulliometry, Ambrose & Ghiassee 1987)
 $\ln(P/\text{kPa}) = 15.09674 - 3599.963/[(T/\text{K}) - 93.307]$, (Antoine eq. from previous comparative ebulliometry measurements, Ambrose & Ghiassee 1987)
 $\log(P_L/\text{kPa}) = 6.50913 - 1542.6/(-94.15 + T/\text{K})$; temp range 355–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.3554 - 2180.05/(-29.337 + T/\text{K})$; temp range 437–592 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 11.53324 - 5291.631/(128.778 + T/\text{K})$; temp range 301–358 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 8.0847 - 3.3219 \times 10^3/(T/\text{K}) + 2.4312 \cdot \log(T/\text{K}) - 1.1734 \times 10^{-2} \cdot (T/\text{K}) + 5.7992 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 268–628 K (vapor pressure eq., Yaws 1994)
 14560* (110.4°C, VLE still-manometry, measured range 110.4–162.9°C, Clifford et al. 2004)
 $\ln(P/\text{kPa}) = 14.511627 - 3164.4707/[(t/^\circ\text{C}) + 156.56122]$; temp range 110.4–162.9°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.0542 (partial pressure, Butler & Ramchandani 1935)
 0.0542; 0.0590; 0.0650 (exptl.; calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)
 0.0375 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 0.0222 (equilibrium partial pressure, Khan & Brimblecombe 1992)
 0.0654 (calculated-bond contribution, Brimblecombe et al. 1992)
 0.358 (calculated-molecular structure, Russell et al. 1992)
 0.0211 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.79 (shake flask-TN, Collander 1951)
 0.94 (calculated-TSA, Iwase et al. 1985)
 0.824, 0.70 (calculated-CLOGP, calculated-M.O., Bodor et al. 1989)
 0.79 (recommended, Sangster 1993)
 0.79 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (2.4 \pm 0.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K was determined using (flash photolysis-resonance fluorescence, Zetzsch & Stuhl 1982; quoted, Atkinson 1985, 1989)

$k(\text{apparent}) \leq 4 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ for reaction with ozone at pH 8 in water, $k \leq 6.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, and $k \leq 6.0 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water at pH 2–4 and 20–23°C (Hoigné & Bader 1983b)

$k_{\text{OH}} = 1.80 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in air and $k(\text{soln}) = 3.70 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the solution-phase reaction with OH radical in aqueous solution (Wallington et al. 1988)

$k_{\text{OH}}(\text{calc}) = 3.11 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.1.4.1

Reported vapor pressures of butyric acid at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log P = A - B/(C + t/^{\circ}C)$		(2)		$\ln P = A - B/(C + t/^{\circ}C)$		(2a)	
$\log P = A - B/(C + T/K)$		(3)		$\ln P = A - B/(C + T/K)$		(3a)	
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Dreisbach & Shrader 1949		Ambrose et al. 1981		Clifford et al. 2004	
summary of literature data		ebulliometry		comparative ebulliometry		VLE still-manometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
25.5	133.3	90.92	4716	76.524	2939	110.4	14560
49.8	666.6	95.01	5704	78.773	3305	117.72	19580
61.5	1333	98.35	6639	81.494	3818	128.17	29650
74.0	2666	101.32	7586	85.202	4614	135.85	39720
88.0	5333	112.57	16500	88.517	5443	141.84	40790
95.5	7999	136.57	42066	92.350	6558	147.07	59860
108.0	13332	150.70	67661	95.880	7754	151.66	69920
125.5	26664	163.25	101326	99.708	9255	155.81	79990
144.5	53329			103.451	10955	159.46	90070
163.5	101325			107.241	13000	161.36	95100
				111.319	15409	162.90	100040
mp/°C	−4.70			115.124	18601		
				120.102	22098	Antoine eq.	
				124.357	26126	eq. 3a	P/kPa
				129.207	31448	A	14.511627
				133.944	37489	B	3164.4707
				144.392	54256	C	156.56122
				149.125	63651		
				154.135	75000	data also fitted to Wagner eq.	
				159.367	89123		
				163.687	101252		
				164.110	102558		
				164.553	103927		
				169.357	120015		
				173.698	136172		
				178.873	157694		
				Antoine eq.			
				eq. 3	P/kPa		
				A	6.55643		
				B	1563.444		
				C	−1563.444		
				data also fitted to Chebyshev and Wagner equations			

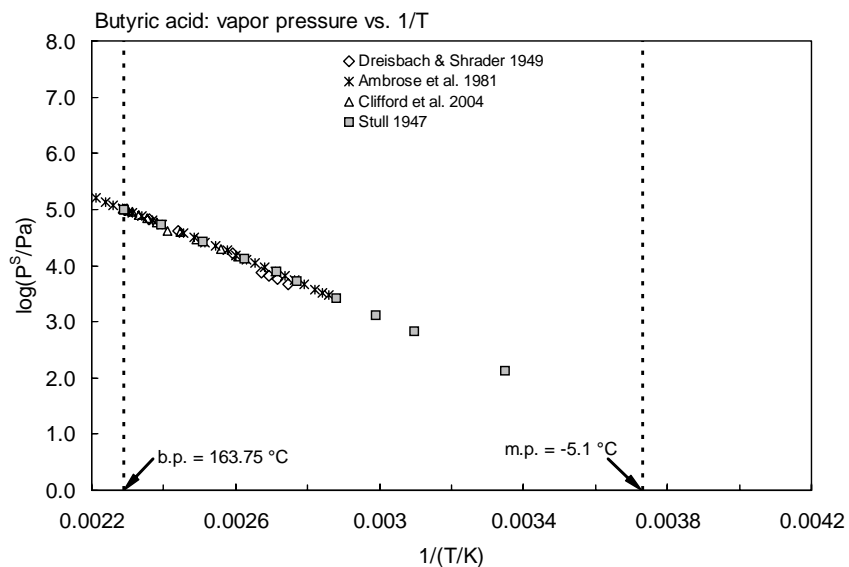
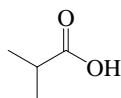


FIGURE 13.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for butyric acid.

13.1.1.5 Isobutyric acid



Common Name: Isobutyric acid

Synonym: isobutanoic acid, *i*-butyric acid, 1-butyric acid, dimethylacetic acid, 2-methylpropionic acid, isopropylformic acid

Chemical Name: *i*-butyric acid, isobutyric acid

CAS Registry No: 79-31-2

Molecular Formula: $C_4H_8O_2$, $(CH_3)_2CHCOOH$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−46.0 (Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

154.45 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9490 (Verschuereen 1983)

0.9682 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

92.7 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

112.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.860 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

5.02 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

228000 ($20^{\circ}C$, synthetic method, Jones 1929)

200000 ($20^{\circ}C$, quoted, Verschuereen 1983)

170000 (Dean 1985)

228000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

273.8* (interpolated-regression of tabulated data, temp range 14.7 – $154.5^{\circ}C$, Stull 1947)

185 (calculated by formula, Dreisbach 1961)

$\log(P/mmHg) = 7.40246 - 1529.2/(185.0 + t/^{\circ}C)$, temp range 73 – $190^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1961)

$\log(P/mmHg) = [-0.2185 \times 11182.8/(T/K)] + 8.55228$; temp range 14.7 – $336^{\circ}C$ (Antoine eq., Weast 1972–73)

185.0 (Riddick et al. 1986)

184* (comparative ebulliometry, measured range 344.3 – $445.6\ K$, Ambrose & Ghassee 1987)

$\ln(P/kPa) = 15.31143 - 3695.332/[(T/K) - 82.0]$; temp range 344.3 – $447\ K$ (Antoine eq. from comparative

ebulliometry measurements, Ambrose & Ghassee 1987)

257.2 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.20794 - 2023.52/(-38.649 + T/K)$; temp range 288 – $428\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.11635 - 2006.61/(-35.297 + T/K)$, temp range 428 – $562\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 11.3037 - 3.1625 \times 10^3/(T/K) + 0.7263 \cdot \log(T/K) - 8.9331 \times 10^{-3} \cdot (T/K) + 4.8215 \times 10^{-6} \cdot (T/K)^2$; temp range 227 – $609\ K$ (vapor pressure eq., Yaws 1994)

14550* ($102.6^{\circ}C$, VLE still-manometer, measured range 102.6 – $153.01^{\circ}C$, Clifford et al. 2004)

$\ln(P/\text{kPa}) = 15.176238 - 3527.8614/[(t/^\circ\text{C}) + 180.5140]$; temp range 102–153.01°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

0.0178, 0.0289, 0.0633 (23.7°C, bubble column technique, concn: 1, 10, 10⁵ ppm. Servant et al. 1991)

0.0897 (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0899 (equilibrium partial pressure, pH 5.4, Khan et al. 1995)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.50, 1.13 (calculated, Verschueren 1983)

0.94 (recommended, Sangster 1993)

1.10 (at pH 3.5, quoted, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}}^* = (2.0 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–440 K (flash photolysis-RF, Dagaut et al. 1988; Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 1.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.1.5.1

Reported vapor pressures of isobutyric acid (2-methyl propanoic acid) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)	$\ln P = A - B/(C + T/K)$		(3a)
$\log P = A - B/(T/K) - C \cdot \log(T/K)$		(4)			
Stull 1947		Ambrose & Giassee 1987		Clifford et al. 2004	
summary of literature data		comparative ebulliometry		VLE still-manometry	
$t/^\circ\text{C}$	P/Pa	T/K	P/Pa	$t/^\circ\text{C}$	P/Pa
14.7	133.3	344.287	3425	102.06	14550
39.3	666.6	347.850	4128	108.99	18580
51.2	1333	350.797	4801	118.62	29650
64.0	2666	355.776	6153	126.28	39720
77.8	5333	357.992	6852	132.29	49790
86.3	7999	360.006	7548	137.60	59850
98.0	13332	361.903	8260	142.36	69920
115.8	26664	365.785	9886	146.62	79990

TABLE 13.1.1.5.1 (Continued)

Stull 1947		Ambrose & Ghiasee 1987		Clifford et al. 2004	
summary of literature data		comparative ebulliometry		VLE still-manometry	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
134.5	53329	369.394	11370	150.21	90070
154.5	101325	375.207	15006	151.71	95100
mp/°C	−47	380.090	18440	153.01	100590
		384.218	21842	Antoine eq. eq. 3(a)	P/kPa
		387.840	25241		
		392.544	30312		
		399.095	38759		
		405.577	48959		
		409.363	55877	A	15.176238
		412.692	62629	B	3527.8614
		↓	↓	C	180.5140
		445.602	172068	data also fitted to Wagner eq.	
		298.15	184		
Antoine eq. eq. 3(a)					
A	15.31143				
B	3695.332				
C	−82.0				
bp/K	427.57				
		data also fitted to Wagner eq.			

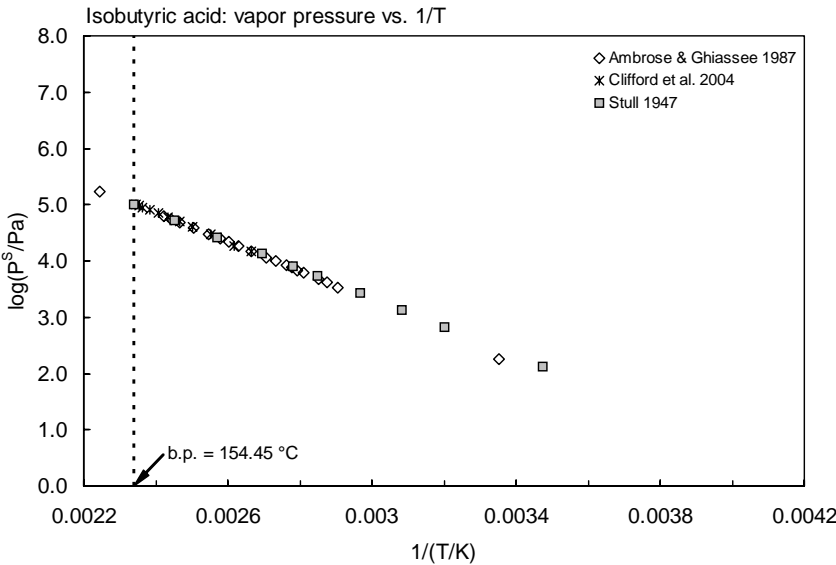
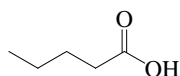


FIGURE 13.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for isobutyric acid.

13.1.1.6 *n*-Valeric acid

Common Name: *n*-Valeric acid

Synonym: pentanoic acid, valeric acid

Chemical Name: *n*-valeric acid, valeric acid

CAS Registry No: 109-52-4

Molecular Formula: C₅H₁₀O₂, CH₃CH₂CH₂CH₂COOH

Molecular Weight: 102.132

Melting Point (°C):

−33.6 (Lide 2003)

Boiling Point (°C):

186.1 (Lide 2003)

Density (g/cm³ at 20°C):

0.9391 (Weast 1982–83)

0.9390 (Dean 1985; Riddick et al. 1986)

Molar Volume (cm³/mol):

108.4 (20°C, calculated-density, Stephenson & Malanowski 1987)

135.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a:

4.820 (18°C, Weast 1982–83)

4.860 (Riddick et al. 1986)

4.830 (Sangster 1989, 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.17 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K, F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

26000 (20°C, quoted, Amidon et al. 1975)

24000 (Verschuereen 1983; Dean 1985)

24000 (20°C, Riddick et al. 1986)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

39.6* (extrapolated-regression of tabulated data, temp range 42.2–184.4°C, Stull 1947)

18.75 (calculated by formula, Dreisbach 1961)

log (P/mmHg) = 7.57366 – 1694.37/(175.0 + t/°C), temp range 102–250°C, (Antoine eq. for liquid state, Dreisbach 1961)

log (P/mmHg) = [−0.2185 × 13370.3/(T/K)] + 9.271178; temp range 42.2–184.4°C (Antoine eq., Weast 1972–73)

20.0 (20°C, Verschuereen 1983)

4.33, 6.37 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 4.58366 – 609.613/(62.754 + t/°C); temp range 72.4–173.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/kPa) = 5.0835 – 878.669/(95.711 + t/°C); temp range 81.1–116.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

log (P/mmHg) = 5.412 – 591/(60 + t/°C); temp range 72–174°C (Antoine eq., Dean 1985, 1992)

19.0 (Riddick et al. 1986)

log (P/kPa) = 6.7818 – 1777.2/(186.6 + t/°C), temp range not specified (Antoine eq., Riddick et al. 1986)

21.0* (comparative ebulliometry, measured range 372.5–465.3 K, Ambrose & Ghassee 1987)

ln (P/kPa) = 15.25555 – 3811.202/[(T/K) – 101.0], temp range 372.5–456.3 K (Antoine eq. from comparative ebulliometry measurements, Ambrose & Ghassee 1987)

16.9 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.69856 - 1694.37/(-98.15 + T/\text{K})$, temp range 375–523 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 15.3454 - 3.9024 \times 10^3/(T/\text{K}) - 0.024353 \cdot \log (T/\text{K}) - 1.1099 \times 10^{-2} \cdot (T/\text{K}) + 5.6315 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 239–651 K (vapor pressure eq., Yaws 1994)

14560 (130°C, VLE still-manometer, measured range 130–178.77°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 36.410366 - 30029.229/(t/^\circ\text{C}) + 760.44819$; temp range 130–178.77°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

0.0478 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

$\ln [K_H' / (\text{mol kg}^{-1} \text{ atm}^{-1})] = -15.37 + 6879/(T/\text{K})$; temp range 278.15–308.15 K. (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0618, 0.0989 (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0448* (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

$\ln [K_H' / (\text{mol kg}^{-1} \text{ atm}^{-1})] = -14.3371 + 6582.96/(T/\text{K})$; temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)

0.0310 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.030 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.861 - 2865/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.42 (Scherrer & Howard 1979)

0.99, 1.69 (calculated, Verschueren 1983)

1.39 (recommended, Sangster 1993)

1.39 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 13.1.1.6.1

Reported vapor pressures and Henry's law constants of n-valeric acid at various temperatures

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)				
$\log P = A - B/(C + T/K)$	(3)	$\ln P = A - B/(C + T/K)$	(3a)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Vapor pressure				Henry's law constant			
Stull 1947		Ambrose & Ghiassaei 1987		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometry		gas stripping	
t/^{\circ}C	P/Pa	T/K	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	H/(Pa m^3/mol)
42.2	133.3	372.543	3410	130.0	14560	5	0.00823
67.7	666.6	376.278	4112	137.56	19590	15	0.018
79.8	1333	379.415	4801	143.92	24630	25	0.0448
93.1	2666	384.489	6125	149.04	29650	35	0.0878

(Continued)

TABLE 13.1.1.6.1 (Continued)

Vapor pressure						Henry's law constant	
Stull 1947		Ambrose & Gdiassee 1987		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometry		gas stripping	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)
116.6	7999	398.670	11637	163.33	49780	ln H = A - B/(T/K)	
128.3	13332	404.759	15006	168.74	59850	H/(mol kg ⁻¹)	
146.0	26664	414.079	21807	173.30	69920	A	-14.3371
165.0	53329	422.753	30285	175.33	74960	B	6582.96
184.4	101325	429.637	55786	17720	79990		
		443.796	62659	17877	86030		
mp/°C	-34.5	449.980	76308				
		454.060	86528	Antoine eq.			
		460.052	101592	eq. 2a	P/Pa		
		405.378	120678	A	36.410366		
				B	30029.229		
				C	760.44819		
		Antoine eq.					
		eq. 2a	P/kPa				
		A	15.2555	data also fitted to Wagner eq.			
		B	3811.202				
		C	-101.0				
		data also fitted to Wagner eq.					

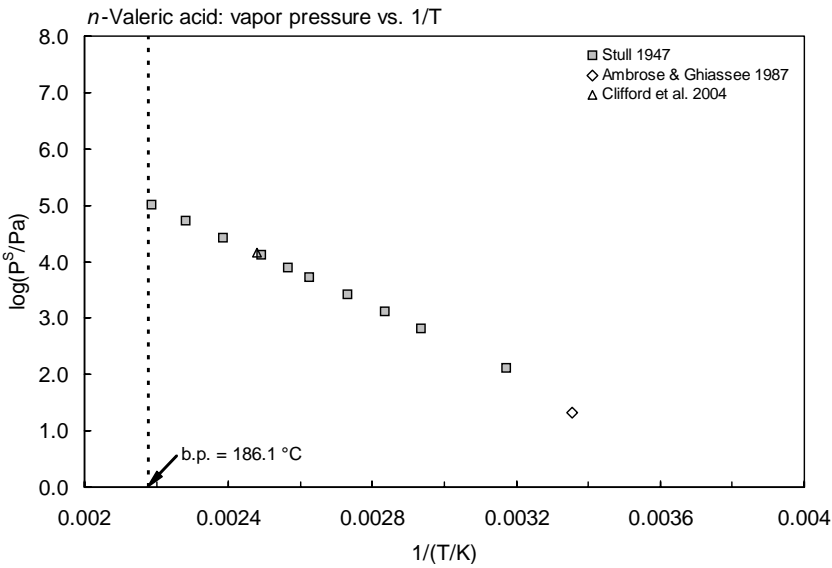


FIGURE 13.1.1.6.1 Logarithm of vapor pressure versus reciprocal temperature for *n*-valeric acid.

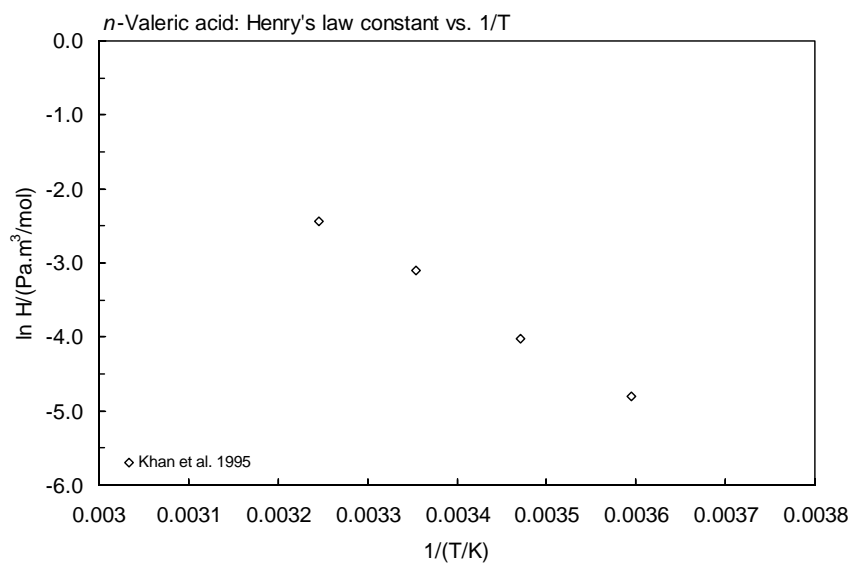
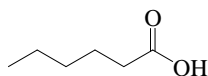


FIGURE 13.1.1.6.2 Logarithm of Henry's law constant versus reciprocal temperature for *n*-valeric acid.

13.1.1.7 Hexanoic acid (Caproic acid)



Common Name: Hexanoic acid

Synonym: butylacetic acid, caproic acid, *n*-hexanoic acid

Chemical Name: butylacetic acid, hexanoic acid, *n*-hexanoic acid

CAS Registry No: 142-62-1

Molecular Formula: $C_6H_{12}O_2$, $CH_3(CH_2)_4COOH$

Molecular Weight: 116.158

Melting Point ($^{\circ}C$):

−3 (Lide 2003)

Boiling Point ($^{\circ}C$):

205.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

125.0 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

157.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.850 (Dean 1985; Bintein & Devillers 1994)

4.879 (Riddick et al. 1986)

4.870 (Sangster 1989, 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.4 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9887 (Valvani et al. 1981)

11000 (Verschuereen 1983)

10816 (Windholz 1983)

6391 (calculated-activity coefficient γ from UNIFAC, Banerjee 1985)

9580 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($71.4^{\circ}C$, summary of literature data, temp range 71.4 – $202^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 16189.4/(T/K)] + 10.431464$; temp range 71.4 – $202^{\circ}C$ (Antoine eq., Weast 1972–73)

4.40 (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.76323 - 1789.425/(T/K) - 101.930$; temp range: 386.3 – $441.8\ K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

26.7 ($20^{\circ}C$, Verschuereen 1983)

9.92, 1.65 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.74777 - 1779.677/(178.361 + t/^{\circ}C)$, temp range 113.1 – $168.6^{\circ}C$ (Antoine eq. from reported exptl. data of Ambrose et al. 1981, Boublik et al. 1984)

$\log(P/kPa) = 6.06182 - 1347.897/(127.391 + t/^{\circ}C)$, temp range 98.1 – $179.1^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/mmHg) = 6.9249 - 1340.8/(126.6 + t/^{\circ}C)$, temp range 98 – $179^{\circ}C$ (Antoine eq., Dean 1985, 1992)

5.00 (Riddick et al. 1986)

$\log(P/kPa) = 6.76323 - 1789.425/(171.22 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

6.0 (calculated from Wagner eq. derived from experimental data, Ambrose & Ghassee 1987)

$\ln(P/kPa) = 15.30352 - 3957.396/[(T/K) - 108]$ (Antoine eq., Ambrose & Ghassee 1987)

$\log(P_L/kPa) = 7.08241 - 2009.93/(-82.69 + T/K)$; temp range 335 – $487\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 55.7058 - 5.6602 \times 10^3/(T/K) - 15.458 \cdot \log (T/K) + 1.0823 \times 10^{-9} \cdot (T/K) + 1.8718 \times 10^{-13} \cdot (T/K)^2$;
temp range 270–667 K (vapor pressure eq., Yaws 1994)

9520 (140.25°C, VLE still-manometer, measured range 140.25–178.28°C, Clifford et al. 2004)

$\ln (P/\text{kPa}) = 13.46595 - 2642.198/[t/^\circ\text{C} + 95.20133]$; temp range 140.25–178.28°C (Antoine eq., VLE still-manometry, Clifford et al. 2004)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0768 (equilibrium partial pressure, pH 1.6–1.9, Khan & Brimblecombe 1992)

$\ln [K_H/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -12.69 + 5988/(T/K)$; temp range 278.15–303.15 K (equilibrium partial pressure, Khan & Brimblecombe 1992)

0.0873, 0.149 (calculated-P/C, calculated-bond contribution, Brimblecombe et al. 1992)

0.0720* (equilibrium partial pressure, pH 5.4, measured range 5–35°C, Khan et al. 1995)

$\ln [K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1})] = -13.9424 + 6303.73/(T/K)$; temp range 5–35°C (equilibrium partial pressure measurements, Khan et al. 1995)

0.0583 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 1996)

0.0556 (20°C, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 3.955 - 2520/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.88 (Scherrer & Howard 1979)

1.87 (HPLC-RT correlation, D'Amboise & Hanai 1982)

1.92 (shake flask-titration, Umland 1983)

2.09 (shake flask-fluorescence, Nishimura et al. 1985)

1.32 (calculated-activity coefficient γ from UNIFAC, Banerjee & Howard 1988)

2.03 ± 0.01 (potentiometric titration, Hersey et al. 1989)

1.92 (recommended, Sangster 1989, 1993)

1.92 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.38; 1.42; 1.57 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)

1.46; 0.88 (soil, quoted exptl.; calculated-MCI χ and fragment contribution, Meylan et al. 1992)

1.46 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 13.1.1.7.1
Reported vapor pressures and Henry's law constants of hexanoic acid (caproic acid) at various temperatures

Vapor pressure						Henry's law constant	
Stull 1947		Ambrose et al. 1981		Clifford et al. 2004		Khan et al. 1995	
summary of literature data		comparative ebulliometry		VLE still-manometer		gas stripping	
t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa	t/°C	H/(Pa m³/mol)
71.4	133.3	386.270	2952	140.25	9520	5	0.0167
89.5	666.6	388.571	3314	149.73	14560	15	0.036
99.5	1333	391.485	3831	156.77	19590	25	0.072
111.8	2666	395.428	4638	162.47	24630	35	0.150
125.0	5333	398.865	5459	166.88	29640		
133.3	7999	402.913	6576	171.11	34680	ln H = A - B/(T/K)	
144.0	13332	406.610	7762	174.73	39720		H/(mol kg ⁻¹)
160.8	26664	410.665	9267	178.28	44750	A	-13.9424
181.0	53329	414.581	10963			B	6303.73
202.0	101325	418.705	13001	Antoine eq.			
		422.887	15422	eq. 2a	P/Pa		
mp/°C	-1.5	432.157	22112	A	13.46595		
		441.779	31458	B	2642.198		
				C	95.20133		
		eq. 2	P/kPa				
		A	6.76323	data also fitted to Wagner eq.			
		B	1789.425				
		C	-101.930				
data also fitted to Wagner eq.							

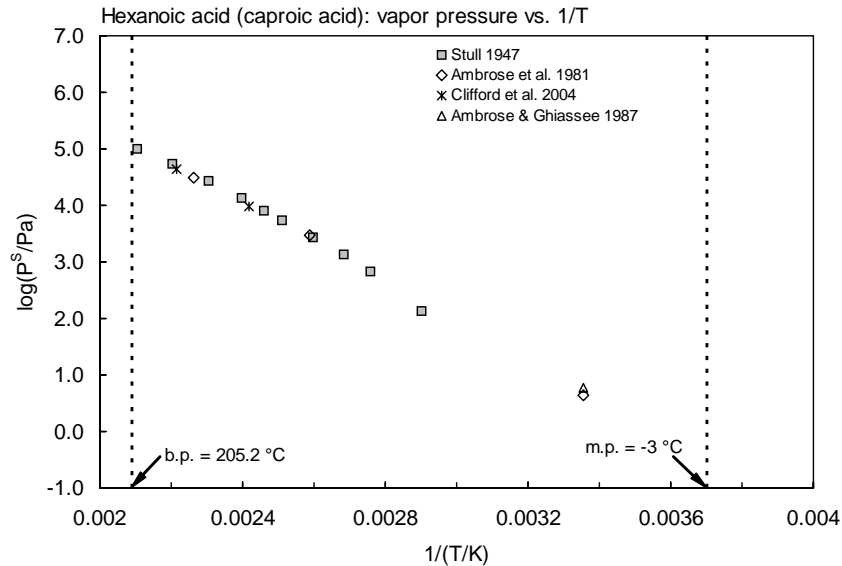


FIGURE 13.1.1.7.1 Logarithm of vapor pressure versus reciprocal temperature for hexanoic acid.

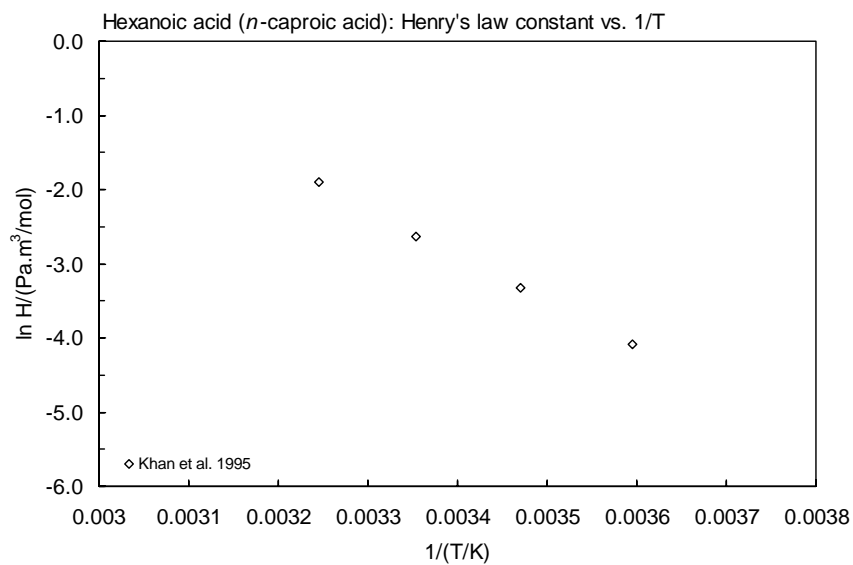
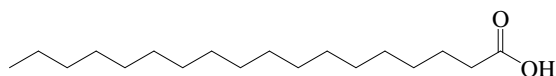


FIGURE 13.1.1.7.2 Logarithm of Henry's law constant versus reciprocal temperature for hexanoic acid.

13.1.1.8 Stearic acid (Octadecanoic acid)



Common Name: Stearic acid

Synonym: octadecanoic acid

Chemical Name: stearic acid, octadecanoic acid, *n*-octadecylic acid

CAS Registry No: 57-11-4

Molecular Formula: $C_{18}H_{36}O_2$, $CH_3(CH_2)_{16}COOH$

Molecular Weight: 284.478

Melting Point ($^{\circ}C$):

69.3 (Lide 2003)

Boiling Point ($^{\circ}C$):

350 (dec., Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9408 (Weast 1982–83)

Molar Volume (cm^3/mol):

335.9 ($70^{\circ}C$, Stephenson & Malanowski 1987)

423.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.50 (estimated, Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

39.57; 43.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.368 (mp at $69.3^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

340 (Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

133.3 ($173.7^{\circ}C$, summary of literature data, temp range: 173.7 – $370^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 19306.6/(T/K)] + 9.457471$; temp range: 173.7 – $370^{\circ}C$, (Antoine eq., Weast 1972–73)

1.69×10^{-12} (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.17126 - 2157.5/(-153.78 + T/K)$; temp range 349 – $415\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.85188 - 1717.93/(-201.829 + T/K)$; temp range 447 – $649\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -40.3638 - 4.7724 \times 10^3/(T/K) + 24.502 \cdot \log(T/K) - 3.7665 \times 10^{-2} \cdot (T/K) + 1.4595 \times 10^{-5} \cdot (T/K)^2$; temp range 343 – $799\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.23 (HPLC-RT correlation, D'Amboise & Hanai 1982)

8.23 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

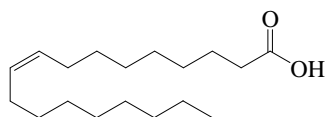
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

13.1.1.9 Oleic acid



Common Name: Oleic acid

Synonym: *cis*-9-octadecenoic acid, (Z)-9-octadecenoic acid

Chemical Name: oleic acid

CAS Registry No: 112-80-1

Molecular Formula: $C_{18}H_{34}O_2$, $CH_3(CH_2)_7CH=CH(CH_2)_6CH_2COOH$

Molecular Weight: 282.462

Melting Point ($^{\circ}C$):

13.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

360 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8870 ($25^{\circ}C$, Riddick et al. 1986)

0.8935 (Lide 2003)

Molar Volume (cm^3/mol):

314.7 (Stephenson & Malanowski 1987)

416.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

5.02 (Riddick et al. 1986)

4.50 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

insoluble (McBain & Richards 1946; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

133 ($178.5^{\circ}C$, summary of literature data, temp range 176.5 – $360^{\circ}C$, Stull 1947)

0.00144 (extrapolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 20326.7/(T/K)] + 9.930301$; temp range 176.5 – $360^{\circ}C$ (Antoine eq., Weast 1972–73)

0.00113 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.22018 - 3711.59/(-36.125 + T/K)$; temp range 444 – 635 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 78.6973 - 8.8227 \times 10^3/(T/K) - 22.472 \cdot \log(T/K) + 4.8353 \times 10^{-11} \cdot (T/K) + 2.6578 \times 10^{-6} \cdot (T/K)^2$; temp range 287 – 633 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

7.64 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)

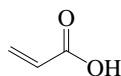
7.64 (recommended, Sangster 1989, 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

13.1.1.10 Acrylic acid (2-Propenoic acid)



Common Name: Acrylic acid

Synonym: acroleic acid, ethylenecarboxylic acid, 2-propenoic acid, propenoic acid

Chemical Name: acrylic acid, 2-propenoic acid, propenoic acid

CAS Registry No: 79-10-7

Molecular Formula: $C_3H_4O_2$, $CH_2=CHCOOH$

Molecular Weight: 72.063

Melting Point ($^{\circ}C$):

12.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

141 (Lide 1003)

Density (g/cm^3 at $20^{\circ}C$):

1.0511 (Weast 1982–83; Dean 1985; Riddick et al. 1986)

Molar Volume (cm^3/mol):

68.9 (calculated-density, Stephenson & Malanowski 1987)\

83.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

–4.41 (Perrin 1972)

4.25 (pK_a , Weast 1982–83)

4.26 (pK_a , Dean 1985)

4.255 (pK_a , Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.13 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

miscible (Riddick et al. 1986)

miscible (Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

570.8 (interpolated-regression of tabulated data, temp range 3.5 – $141^{\circ}C$, Stull 1947)

506.5 (Hoy 1970)

570 (interpolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 10955.1/(T/K)] + 8.659704$; temp range 3.5 – $141^{\circ}C$ (Antoine eq., Weast 1972–73)

426.6 ($20^{\circ}C$, Verschueren 1983)

$\log(P/mmHg) = 5.65204 - 648.629/(154.683 + t/^{\circ}C)$; temp range 20 – $70^{\circ}C$ (Antoine eq., Dean 1985, 1992)

533.0 (Howard et al. 1986)

1030 ($20^{\circ}C$, Riddick et al. 1986)

581.7 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.93296 - 1827.9/(-43.15 + T/K)$; temp range 341 – $414\ K$ (Antoine eq., Stephenson & Malanowski 1987)

533, 12530 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/mmHg) = 23.0607 - 3.1347 \times 10^3/(T/K) - 4.8813 \cdot \log(T/K) + 4.369 \times 10^{-4} \cdot (T/K) - 4.9161 \times 10^{-13} \cdot (T/K)^2$; temp range 287 – $615\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

0.042 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 0.43 (Leo et al. 1971)
- 0.31, 0.43 (calculated, Verschueren 1983)
- 0.35 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} t_{1/2} = 2.5\text{--}23.8$ h in air, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous screening test data (Dore et al. 1975; Sasaki 1978; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672\text{--}4320$ h, based on unacclimated anaerobic reactor test data (Chou et al. 1979; selected, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 28$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.5\text{--}23.8$ h, based on an estimated rate constant for the vapor-phase reaction with hydroxyl radical and ozone in air (Atkinson & Carter 1984; Atkinson 1987; selected, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 28$ d in natural waters (Capel & Larson 1995)

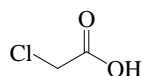
Groundwater: $t_{1/2} = 48\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

13.1.1.11 Chloroacetic acid



Common Name: Chloroacetic acid

Synonym:

Chemical Name: chloroacetic acid (α or β)

CAS Registry No: 79-11-8

Molecular Formula: $\text{C}_2\text{H}_3\text{ClO}_2$, ClCH_2COOH

Molecular Weight: 94.497

Melting Point ($^{\circ}\text{C}$):

61.2 (α , Stull 1947; Yalkowsky & Valvani 1980)

56.0 (β , Yalkowsky & Valvani 1980)

56–63 (Weast 1982–83; Dean 1985)

63 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

189.3 (Lide 2003)

Density (g/cm^3 at 20°C):

1.4043 (40°C , Weast 1982–83)

Molar Volume (cm^3/mol):

68.8 (63°C , Stephenson & Malanowski 1987)

89.3 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.85 (Weast 1982–83)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

56 (estimated, Yalkowsky & Valvani 1980)

36.73, 42.22 (observed for α , observed for β , Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 0.424 (mp at 63°C)

Water Solubility (g/m^3 or mg/L at 25°C):

120835 (α , calculated- ΔS_{fus} and mp, calculated-mp, Yalkowsky & Valvani 1980)

107200 (β , calculated- ΔS_{fus} and mp, calculated-mp, Yalkowsky & Valvani 1980)

109000 (shake flask-titrimetric assay, Bowden et al. 1998)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

39.70* (extrapolated-regression of tabulated data, temp range 43.0 – 189.5°C , Stull 1947)

$\log(P/\text{mmHg}) = 8.28534 - 2263.7/(230 + t/^{\circ}\text{C})$ (Antoine eq., Dreisbach & Martin 1949)

6301* (112.8°C , ebulliometry, measured range 112.8 – 187.55°C , Dreisbach & Shrader 1949)

4141* (104.47°C , ebulliometry, measured range 104.47 – 190.27°C , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 7.56597 - 1733.96/(180.996 + t/^{\circ}\text{C})$; temp range: 104 – 190°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)

$\log(P/\text{mmHg}) = [-0.2185 \times 13134.5/(T/\text{K})] + 9.099371$; temp range 43 – 189°C (Antoine eq., Weast 1972–73)

18.52, 12.9 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.67559 - 1723.714/(180.01 + t/^{\circ}\text{C})$; temp range 104 – 190.27°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.29612 - 1468.443/(154.397 + t/^{\circ}\text{C})$; temp range 123.19 – 187.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

18.52 (extrapolated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.55016 - 1723.365/(179.98 + t/^{\circ}\text{C})$; temp range 104 – 190°C (Antoine eq., Dean 1985, 1992)

8.51, 11.5 (extrapolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.69087 - 1733.96/(-92.154 + T/\text{K})$; temp range 336–463 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.67975 - 1727.293/(-97.742 + T/\text{K})$; temp range 377–464 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 42.6726 - 4.597 \times 10^3/(T/\text{K}) - 11.348 \cdot \log (T/\text{K}) - 2.8515 \times 10^{-10} \cdot (T/\text{K}) + 1.7995 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 333–686 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

0.000938 (partial pressure equilibrium, Bowden et al. 1998)

$\ln [(K_H'/(\text{mol kg}^{-1} \text{ atm}^{-1}))] = -21.087 + 9742.6/(T/\text{K})$, temp range $5\text{--}35^\circ\text{C}$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000536 (20°C , selected from literature experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 7.343 - 4104/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.22 (shake flask, Hansch & Leo 1987; recommended, Hansch et al. 1995)

0.22 (recommended, Sangster 1993)

0.22 (calculated-fragment const. with correction factors in multiCASE program, Dambrosky et al. 2001)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: aqueous photolysis $t_{1/2} = 1900\text{--}19000$ h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991);

atmospheric photolysis $t_{1/2} = 1900\text{--}19000$ h, based on estimated aqueous photolysis half-life (Howard et al. 1991);

photocatalyzed mineralization by the presence of TiO_2 with the rate of 5.5 ppm/min per gram of catalyst (Ollis 1985).

Hydrolysis: first-order hydrolysis $t_{1/2} = 23000$ h, based on losses in dark control tests during photolysis experiments (Draper & Crosby 1983; quoted, Howard et al. 1991).

Oxidation: photooxidation $t_{1/2} = 230\text{--}2300$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on river die-away tests using radio-labeled material (Boethling & Alexander 1979; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 230\text{--}2300$ h, based on estimated rate constant for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 5 d (Kelly et al. 1994).

Surface water: aqueous photolysis $t_{1/2} = 1900\text{--}19000$ h, based on experimental photolysis data utilizing an artificial light source (Draper & Crosby 1983; quoted, Howard et al. 1991); $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 13.1.1.11.1

Reported vapor pressures of chloroacetic acid at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Dreisbach & Shrader 1949		McDonald et al. 1959	
summary of literature data		ebulliometry		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
43.0	133	112.8	6301	104.47	4141
68.3	666.6	123.19	10114	114.60	6675
81.0	1333	134.67	16468	128.32	12103
94.2	2666	159.95	42066	146.78	25198
109.2	5333	174.44	67661	167.51	38583
118.3	7999	187.55	101325	187.59	97205
130.7	13332			189.35	102165
140.0	26664			190.27	104738
169.0	53329				
189.5	101325			mp/°C	62.65
mp/°C	61.2			eq. 2	P/mmHg
				A	7.56597
				B	1733.96
				C	180.996

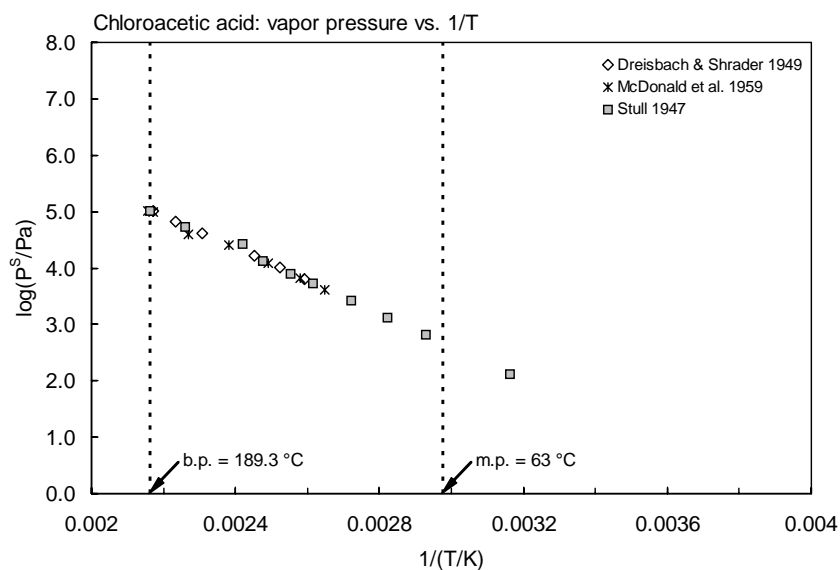
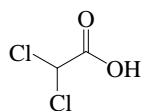


FIGURE 13.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for chloroacetic acid.

13.1.1.12 Dichloroacetic acid



Common Name: Dichloroacetic acid

Synonym: dichloroethanoic acid

Chemical Name: dichloroacetic acid

CAS Registry No: 79-43-6

Molecular Formula: $C_2H_2Cl_2O_2$, $Cl_2CHCOOH$

Molecular Weight: 128.942

Melting Point ($^{\circ}C$):

13.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

194.0 (Weast 1982–83; Verschueren 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5634 (Weast 1982–83)

1.5630 (Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

82.50 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

110.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

1.26 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

miscible (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

37.94* (extrapolated-regression of tabulated data, temp range 44 – $194.4^{\circ}C$, Stull 1947)

133.3 ($44^{\circ}C$, Stull 1947; quoted, Verschueren 1983)

$\log(P/mmHg) = [-0.2185 \times 12952.9/(T/K)] + 8.946605$; temp range 44 – $194.4^{\circ}C$ (Antoine eq., Weast 1972–73)

34.3 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.47122 - 2385.6/(-31.197 + T/K)$, temp range 317 – $468\ K$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = -7.2806 - 3.3706 \times 10^3/(T/K) + 9.3771 \cdot \log(T/K) - 2.0832 \times 10^{-2} \cdot (T/K) + 9.5091 \times 10^{-6} \cdot (T/K)^2$; temp range 287 – $686\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.00085 (partial pressure equilibrium, Bowden et al. 1998)

$\ln[(K_H'/(mol\ kg^{-1}\ atm^{-1}))] = -15.1776 + 8010.6/(T/K)$; temp range 5 – $35^{\circ}C$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000536 ($20^{\circ}C$, selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 4.776 - 3352/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.92 (shake flask, Log P Database, Hansch & Leo 1987)

0.92 (recommended, Sangster 1993)

0.92 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photocatalyzed mineralization by the presence of TiO_2 with the rate of 8.5 ppm/min per gram catalyst (Ollis 1985).

Half-Lives in the Environment:

TABLE 13.1.1.12.1

Reported vapor pressures of dichloroacetic acid at various temperatures

Stull 1947

summary of literature data

$t/^{\circ}C$	P/Pa
44.0	133
69.8	666.6
82.6	1333
96.3	2666
111.8	5333
121.5	7999
134.0	13332
152.3	26664
173.7	53329
194.4	101325
mp/ $^{\circ}C$	9.7

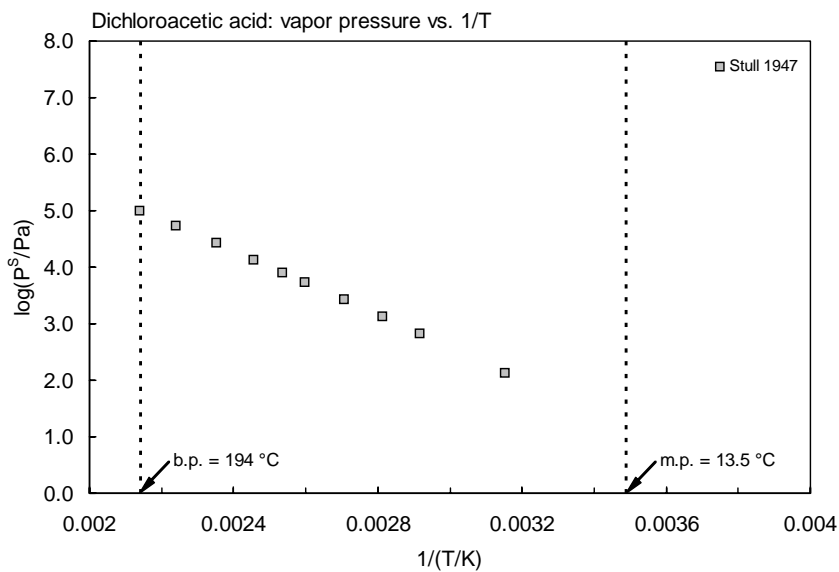
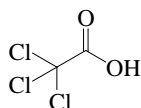


FIGURE 13.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for dichloroacetic acid.

13.1.1.13 Trichloroacetic acid



Common Name: Trichloroacetic acid

Synonym: TCA

Chemical Name: trichloroacetic acid (α or β)

CAS Registry No: 76-03-9

Molecular Formula: Cl_3CCOOH

Molecular Weight: 163.39

Melting Point ($^{\circ}\text{C}$):

59.2 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

196.5 (Lide 2003)

Density (g/cm^3 at 20°C):

1.620 (25°C , Weast 1982–83)

Molar Volume (cm^3/mol):

100.3 (61°C , Stephenson & Malanowski 1987)

131.1 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

0.70 (Weast 1982–83)

0.52 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

17.78, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 0.462 (mp at 59.2°C)

Water Solubility (g/m^3 or mg/L at 25°C):

114550 (calculated- ΔS_{fus} and mp, Yalkowsky & Valvani 1980)

191860 (calculated-mp, Yalkowsky & Valvani 1980)

13000 (Verschueren 1983)

1200000 (120 in 100 parts solvent, Dean 1985)

38300 (calculated-group contribution method, Kühne et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

21.88* (extrapolated-regression of tabulated data, temp range 51 – 195.6°C , Stull 1947)

4620* (112.62°C , ebulliometry, measured range 112.62 – 197.93°C , McDonald et al. 1959)

$\log(P/\text{mmHg}) = 7.31057 - 1618.97/(167.882 + t/^{\circ}\text{C})$; temp range 112.6 – 197.94°C (Antoine eq. from ebulliometry measurement, McDonald et al. 1959)

$\log(P/\text{mmHg}) = [-0.2185 \times 13817.0/(T/\text{K})] + 9.341430$; temp range 51 – 195.6°C (Antoine eq., Weast 1972–73)

10.63 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/\text{kPa}) = 6.4026 - 1597.434/(165.711 + t/^{\circ}\text{C})$; temp range 112.6 – 197.93°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)

66.14 (extrapolated-Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 7.2730 - 1594.3/(165.4 + t/^{\circ}\text{C})$; temp range 112 – 198°C (Antoine eq., Dean 1985, 1992)

133.3 (Howard et al. 1986; quoted, Banerjee et al. 1990)

11.01 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.43547 - 1618.97/(-105.268 + T/\text{K})$; temp range 326 – 473 K (Antoine eq., Stephenson & Malanowski 1987)

133.3, 491 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)

$\log(P/\text{mmHg}) = 63.4449 - 3.6769 \times 10^3/(T/\text{K}) - 21.13 \cdot \log(T/\text{K}) + 1.0777 \times 10^{-2} \cdot (T/\text{K}) + 4.8481 \times 10^{-12} \cdot (T/\text{K})^2$; temp range 258 – 491 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.000137 (partial pressure equilibrium, Bowden et al. 1998)

$\ln [(K_H'/(\text{mol kg}^{-1} \text{atm}^{-1}))] = -17.836 + 8660.09/(T/K)$; temp range $5\text{--}35^\circ\text{C}$ (partial pressure equilibrium measurements, Bowden et al. 1998)

0.000834 (20°C , selected from literature, experimentally measured data, Staudinger & Roberts 2001)

$\log K_{AW} = 5.931 - 3634/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.33 (shake flask, Log P Database, Hansch & Leo 1987)

1.33 (recommended, Sangster 1993)

1.33 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: no photocatalyzed mineralization by the presence of TiO_2 as compared to both dichloroacetic acid and trichloroacetic acid (Ollis 1985).

Half-Lives in the Environment:

TABLE 13.1.1.13.1

Reported vapor pressures of trichloroacetic acid at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$	(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)		
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)		
Stull 1947		McDonald et al. 1959		
summary of literature data		ebulliometry		
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	
51.0	133	112.62	4620	
76.0	666.6	118.13	5949	
88.2	1333	122.75	7326	
101.8	2666	129.99	9998	
116.3	5333	168.75	42302	
125.9	7999	183.92	68210	
137.8	13332	194.91	94156	
155.4	26664	196.49	98175	
175.2	53329	197.02	99584	
195.6	101325	197.48	100901	
		197.93	102318	
mp/ $^\circ\text{C}$	57.0	mp/ $^\circ\text{C}$	59.16	
		eq. 2	P/mmHg	
		A	7.31057	
		B	1618.97	
		C	167.882	

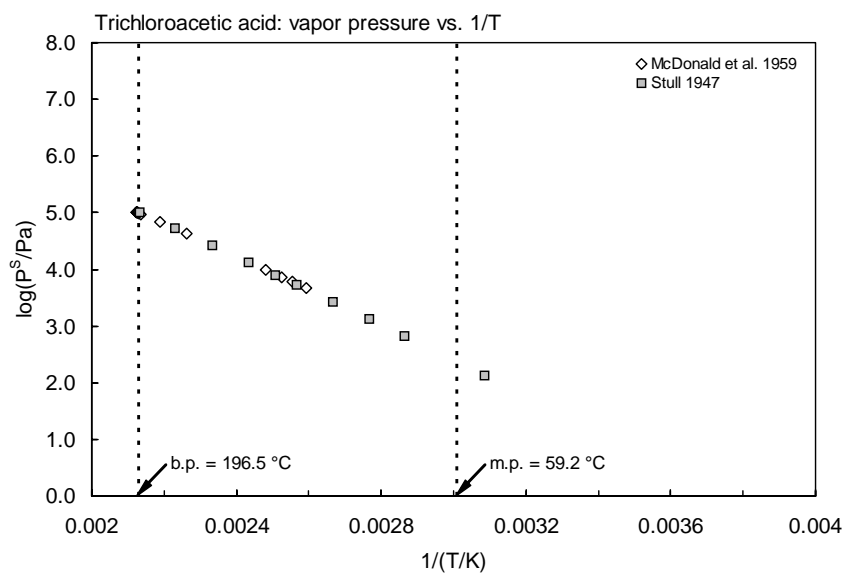
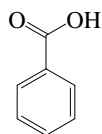


FIGURE 13.1.13.1 Logarithm of vapor pressure versus reciprocal temperature for trichloroacetic acid.

13.1.2 AROMATIC ACIDS**13.1.2.1 Benzoic acid**

Common Name: Benzoic acid

Synonym:

Chemical Name: benzoic acid

CAS Registry No: 65-85-0

Molecular Formula: $C_7H_6O_2$, C_6H_5COOH

Molecular Weight: 122.122

Melting Point ($^{\circ}C$):

122.35 (Lide 2003)

Boiling Point ($^{\circ}C$):

249.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.2659 ($15^{\circ}C$, Weast 1982–83)

1.0800 (Dean 1985)

Molar Volume (cm^3/mol):

113.6 ($130^{\circ}C$, Stephenson & Malanowski 1987)

134.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.20 (McDaniel & Brown 1958)

4.33 ± 0.02 , 4.38 ± 0.03 (HPLC, Unger et al. 1978)

4.08 (shake flask-TN, Clarke 1984)

4.05 ± 0.01 (equilibrium titration, Clarke & Cahoon 1987)

4.204 (Dean 1985; Lee et al. 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

69.2 (395.2 K, de Kruif & Block 1982)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

94.5 ($25^{\circ}C$, average value, Malaspina et al. 1973)

90.6 (Colomina et al. 1982)

90.51 (Ribeiro da Silva et al. 1995)

89.71 (Li et al. 2002)

90.1 (Li et al. 2004)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.0 (Tsonopoulos & Prausnitz 1971)

18.2 (395.2 K, de Kruif & Block 1982)

Entropy of Fusion, ΔS_{fus} (J/mol K):

45.61 (Tsonopoulos & Prausnitz 1971)

43.81 (Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.111 (mp at $122.35^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3340* ($24.6^{\circ}C$, shake flask-synthetic method, Ward & Cooper 1930)

3298* (shake flask-thermostatic and synthetic methods, measured range 25 – $88.6^{\circ}C$, Morrision 1944)

4200 (shake flask-liquid scintillation counting, Lu & Metcalf 1975)

3600 (shake flask-UV, Yalkowsky et al. 1983)

3416* (shake flask-weight titration, measured temp range 5 – $65^{\circ}C$, Strong et al. 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 799.9* (122.2°C, static method-manometer, measured range 122.2–249.0°C, Kahlbaum 1898)
 6.893* (60.1°C, isoteniscope method, measured range 60.1–247°C, Klosky et al. 1927)
 $\log(P_s/\text{mmHg}) = 11.956 - 4409/(T/K)$; temp range 61–121°C (solid, isoteniscope, Klosky et al. 1927)
 $\log(P_L/\text{mmHg}) = 30.172 - 4714/(T/K) - 6.720 \cdot \log(T/K)$; temp range 128–247°C (liquid, isoteniscope, Klosky et al. 1927)
 0.840* (extrapolated-regression of tabulated data, temp range 96–227°C, Stull 1947)
 12.35* (70.48°C, transpiration method, measured range 70.48–114.11°C, Davies & Jones 1954)
 $\log(P/\text{mmHg}) = 12.8699 - 4775.7/(T/K)$, temp range 70.48–114.11°C (transpiration, Davies & Jones 1954)
 0.160* (298.3 K, Knudsen effusion, measured range 290.4–315.5 K, Wiedemann 1971)
 $\log(P/\text{mmHg}) = [-0.2185 \times 15253.3/(T/K)] + 9.03300$; temp range 60–110°C (Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 16295.1/(T/K)] + 9.741362$; temp range 96–249.2°C (Antoine eq., Weast 1972–73)
 0.160* (Knudsen effusion weight-loss method, fitted to Antoine eq., measured range 65.05–110.25°C, Malaspina et al. 1973)
 $\log(P/\text{mmHg}) = (12.175 \pm 0.040) - (4501 \pm 17)/(T/K)$; temp range 338–383 K (Antoine eq., Knudsen effusion, Malaspina et al. 1973)
 0.108* (effusion method, measured range 25–70.5°C, DePablo 1976)
 16.8* (71.25°C, isoteniscope method, measured range 344.4–393.8 K, Sachinidis & Hill 1980)
 $\log(P/\text{mmHg}) = 12.45 - 4605/(T/K)$; temp range 344.4–393.8 K (isoteniscope method, Sachinidis & Hill 1980)
 0.070*, 0.050* (20°C, gas saturation method, vapor pressure balance, OECD 1981)
 0.112* (25.25°C, Knudsen effusion method, temp range 20.25–40.25°C, Colomina et al. 1982)
 $\log(P/\text{Pa}) = (14.87 \pm 0.02) - (4719.6 \pm 7.1)/(T/K)$; temp range 293.4–313.4 K (Antoine eq., Knudsen effusion, Colomina et al. 1982)
 0.0907 (20°C, evaporation method, Gückel et al. 1982)
 0.105* (diaphragm manometer/torsion mass-loss effusion, extrapolated from measured range 316–391 K, de Kruif & Block 1982)
 0.109 ± 0.005 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
 0.9505 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 9.033 - 3333.3/(T/K)$, temp range 60–110°C (Antoine eq., Dean 1985, 1992)
 0.105 (solid P_s , interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 15.94025 - 7420.596/(74.333 + T/K)$; temp range 294–321 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 11.8285 - 4719.5/(T/K)$; temp range 343–373 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
 0.772 (liquid P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.80911 - 2776.12/(-43.978 + T/K)$; temp range 405–523 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
 0.600 (20°C, OECD 1981; quoted, Howard 1989)
 $\log(P/\text{mmHg}) = -140.0388 + 80.479/(T/K) + 62.611 \cdot \log(T/K) - 6.5321 \times 10^{-2} \cdot (T/K) + 2.4596 \times 10^{-5} \cdot (T/K)^2$; temp range 396–751 K (vapor pressure eq., Yaws 1994)
 0.13* (26°C, Knudsen effusion, measured range 26–50°C, Li et al. 2002)
 $\ln(P/\text{Pa}) = (34.031 \pm 0.30) - (10790 \pm 93)/(T/K)$; temp range 299–323 K (Knudsen effusion technique, Li et al. 2002)
 $\ln(P/\text{Pa}) = 34.320 - 10866/(T/K)$; temp range 304–317 K (regression eq. of Ribeiro da Silva et al. 1995 data, Li et al. 2004)
 $\ln(P/\text{Pa}) = (34.181 \pm 0.446) - (10836 \pm 140)/(T/K)$; temp range 299–328 K (Knudsen effusion technique, Li et al. 2004)

Henry's Law Constant (Pa m³/mol at 25°C):

- 0.00709 (Howard 1989)
 0.00575; 0.0110 (calculated-P/C, calculated-bond contribution, Meylan & Howard 1991)
 0.00415 (computed-vapor liquid equilibrium VLE data, Yaws et al. 1991)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 1.87 (shake flask-UV, Fujita et al. 1964)
- 1.68 (shake flask-UV, Halmekoski & Hannikainen 1964)
- 1.85 \pm 0.01 (shake flask-UV, Iwasa et al. 1965)
- 2.03 (shake flask-LSC, Lu & Metcalf 1975)
- 1.78 \pm 0.01, 1.77 \pm 0.01 (HPLC- k' correlation, Unger et al. 1978)
- 1.79 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
- 1.86, 1.87 (calculated-fragment const., Rekker 1977)
- 1.94 (RP-HPLC correlation, Hanai & Hubert 1982)
- 1.95 (HPLC- k' correlation; Miyake & Terada 1982)
- 1.87 (microelectrometric titration, Clarke 1984)
- 2.18 \pm 0.03; 2.03 (exptl.-ALPM, selected best lit. value, Garst & Wilson 1984)
- 1.44, 1.87 (HPLC- k' correlation, Haky & Young 1984)
- 1.88 (shake flask-UV at pH 0.5, Nishimura et al. 1985)
- 1.97 (microelectrometric titration, Clarke & Cahoon 1987)
- 1.94 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
- 1.93 (HPLC- k' correlation, Miyake et al. 1987)
- 1.88 (CPC, Berthod et al. 1988)
- 1.85 \pm 0.04 ("Filter Chamber"-UV, Hersey et al. 1989)
- 1.87 (recommended, Sangster 1989, 1993)
- 1.88 (back flashing-CPC centrifugal partition chromatography, Menges et al. 1990)
- 1.87 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:

- 1.32, 2.00, 2.14 (fish, algae, mosquito, Lu & Metcalf 1975)
- 3.26, 3.45 (daphnia, snail, Lu & Metcalf 1975)
- 0.48 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
- 1.43 (alga *Chlorella fusca*, calculated- K_{ow} , Geyer et al. 1984)
- < 1.0 (golden ide, Freitag et al. 1985)
- < 1.0 (algae, Freitag et al. 1985)
- 3.11 (activated sludge, Freitag et al. 1985)
- 1.15 (trout muscle, calculated- K_{ow} , Branson 1978)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.26; 1.86; 0.602 (Alfisol soil; Podzol soil; sediment, von Oepen et al. 1991)
- 1.50 (soil, quoted exptl., Meylan et al. 1992)
- 1.16 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
- 1.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: rate of evaporation $k = 1.89 \times 10^{-8} \text{ mol cm}^{-2} \text{ h}^{-1}$ at 20°C determined by evaporation method (Gückel et al. 1982).

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.0 \text{ d}$, based on estimated vapor-phase reaction with hydroxyl radical in air (Howard 1989).

Hydrolysis: $k = 4.3 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ for reactions of hydroxyl radical in aqueous solution (Buxton et al. 1986)

$k = 1.15 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ (Mabury & Crosby 1996);

$k(\text{exptl}) = 1.2 \times 10^{13} \text{ M}^{-1} \text{ h}^{-1}$ for reaction with hydroxy radical (Armbrust 2000)

Biodegradation: completely degraded by a soil microflora after 24 h (Alexander & Lustigman 1966; quoted, Verschueren 1983);

completely degraded for 16 mg/L concn. within one day by soil and by wastewater (Haller 1978);

$t_{1/2} \sim 0.2\text{--}3.6$ d if released into water, should readily biodegrade (Howard 1989);
average $k(\text{exptl}) = 0.11533 \text{ h}^{-1}$ compared to group method predicted $k = 0.0993 \text{ h}^{-1}$ (nonlinear) and $k = 0.0263 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).
Biotransformation: degradation $k = 6.84 \times 10^{-17} \text{ mol cell}^{-1} \text{ h}^{-1}$ in pure culture system (Banerjee et al. 1984).
Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} \sim 2.0$ d for reactions with photochemically produced hydroxyl radical (Howard 1989).
Surface water: if released into water, should readily biodegrade with an estimated $t_{1/2} = 0.2\text{--}3.6$ d (Howard 1989).
Groundwater:
Sediment:
Soil:
Biota:

TABLE 13.1.2.1.1
Reported aqueous solubilities of benzoic acid at various temperatures

Ward & Cooper 1930		Morrison 1944		Strong et al. 1989	
shake flask-synthetic method		thermostatic and synthetic		shake flask-weight titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
24.6	3340	25.0	3298	5	1830
42.4	6280	35.0	4641	15	2482
57.8	10930	45.0	6167	25	3416
74.1	20670	55.4	10137	35	4776
83.1	31300	60.2	12213	45	6656
88.3	39660	64.6	14533	55	9629
		68.5	16976	65	14325
		75.1	22838		
		79.3	26991	$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 23.29$ 25°C	
		82.1	31021		
		88.6	43356		

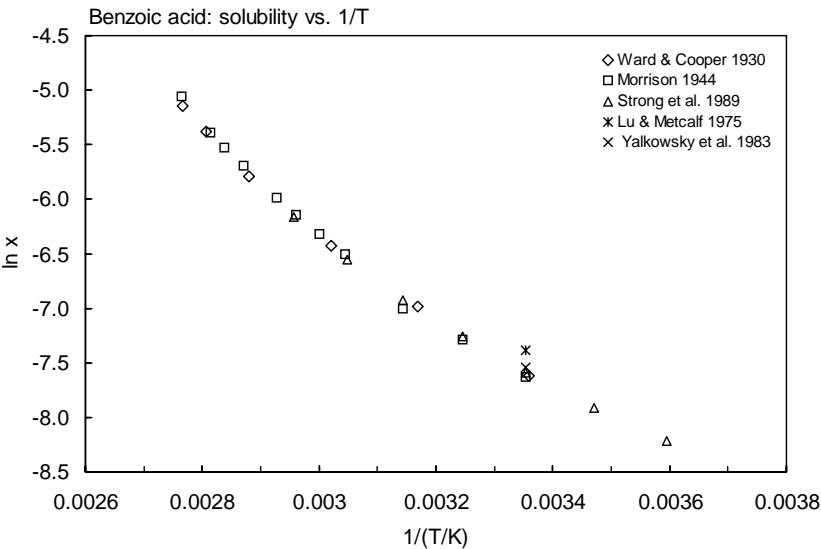


FIGURE 13.1.2.1.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for benzoic acid.

TABLE 13.1.2.1.2

Reported vapor pressures of benzoic acid at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & \end{aligned}$$

1.

Kahlbaum 1898		Klosky et al. 1927		Stull 1947		Davies & Jones 1954	
static method-manometer*		isoteniscope method		summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
			solid				
122.2	799.9	60.1	6.893	96.0	133.3	70.48	12.35
132.5	1333	80.4	41.06	119.5	666.6	75.14	19.33
146.5	2666	100.2	190.1	132.1	1333	80.43	31.02
155.5	4000	121.0	777.3	146.7	2666	84.47	44.0
161.9	5333			162.6	5333	89.88	68.66
167.2	6666	eq. 1	P/mmHg	172.8	7999	95.35	108.9
178.5	9999	A	11.956	186.2	13332	100.59	149.2
185.9	13332	B	4409	205.8	26664	105.05	230.8
196.5	19998			227.0	53329	109.85	341.0
204.9	26664		liquid	249.2	101325	114.11	458.1
211.5	33331	128.6	1120				
217.0	39997	134.5	1573	mp/°C	121.7	eq. 1	P/mmHg
225.8	53329	148.0	2960			A	12.8699
233.8	66661	158.2	4533			B	4775.7
239.8	79993	172.8	8506				
245.5	93326	187.6	14772			$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 91.42$	
249.0	101325	199.7	22238			at 365.5 K	
		216.2	38224			$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 94.37$	
		233.0	63835			at 298.15 K	
		247.0	95739				
		eq. 4	P/mmHg				
		A	30.172				
		B	4714				
		C	6.720				

*complete list see [ref.](#)

2.

Wiedemann 1971		Malaspina et al. 1973		Sachinidis & Hill 1980		OECD 1981	
Knudsen effusion		Knudsen effusion		isoteniscope-manometer		gas saturation/effusion	
T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
					gas saturation		
290.4	0.0613	65.05	9.879	344.4	16.80	10	0.02
294.4	0.118	71.35	16.72	352.8	37.73	20	0.07
298.3	0.160	74.65	23.91	373.7	167.6	30	0.24
299.8	0.205	77.95	29.69	393.8	733.5	40	0.76
300.5	0.244	85.25	55.02			50	2.20
301.1	0.220	89.15	76.1	eq. 1	P/mmHg	vapor pressure balance	
304.4	0.337	94.05	112.5	A	12.45	10	0.012
315.5	1.173	99.75	169.2	B	4605	20	0.05

TABLE 13.1.2.1.2 (Continued)

Wiedemann 1971		Malaspina et al. 1973		Sachinidis & Hill 1980		OECD 1981	
Knudsen effusion		Knudsen effusion		isoteniscope-manometer		gas saturation/effusion	
T/K	P/Pa	t/°C	P/Pa	T/K	P/Pa	t/°C	P/Pa
293.36	0.0889*	105.05	255.3	$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 88.1$		30	0.17
293.56	0.0907*	110.25	362.7			40	0.56
293.36	0.0893*					50	1.70
		$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.92$		<div>DePablo 1976</div> <div>effusion method</div>			
eq. 1	P/mmHg	at 298.15 K					
A	12.2937	$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 86.18$					
B	4530.02	at 360.8 K					
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 86.61$		eq. 1	P/mmHg				
		A	12.175	25	0.108		
*different orifice areas of Knudsen effusion cell		B	4501	45	1.03		
		temp range 338.2–383.4 K		70.25	11.92		
		calculated average value					
		$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 94.5$					
		at 298 K					

3.

Colomina et al. 1982		de Kruif & Block 1982		Li et al. 2002	
Knudsen effusion		manometer/effusion		Knudsen effusion	
T/K	P/Pa	T/K	P/Pa	T/K	P/Pa
293.4	0.0604	316.4	0.89	299.15	0.13
293.67	0.063	321.01	1.44	303.25	0.22
295.5	0.0781	321.25	1.48	308.15	0.38
295.75	0.0814	323.58	1.9	313.15	0.66
296.59	0.09	328.73	3.25	318.15	1.13
298.38	0.112	329.01	3.34	323.15	1.86
298.95	0.119	335.67	6.44		
301.19	0.157	338.66	8.6	eq. 1a	P/Pa
301.71	0.167	344.64	14.74	A	34.031
304.47	0.23	347.6	19.6	B	10790
305.15	0.25	350.01	24.17		
307.6	0.334	353.14	31.79		
308.11	0.354	359.05	52.37		
308.34	0.365	361.41	63.5		
310.14	0.445	364.96	84.69		
311.17	0.503	367.77	106.4		
311.29	0.508	368.43	111.9		
313.38	0.64	383.04	334.8		
		390.93	588.4		
eq. 1	P/Pa	Data fitted to 3-parameter vapor-pressure eq. see ref. at 395.52K			
A	14.87				
B	4719.6				
$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 90.6 \pm 0.2$		$\Delta H_{\text{v}}/(\text{kJ/mol}) = 69.2$			
temp range 293–313 K		$\Delta H_{\text{subl}}/(\text{kJ/mol}) = 87.4$			
		$\Delta H_{\text{fus}}/(\text{kJ/mol}) = 18.0$			

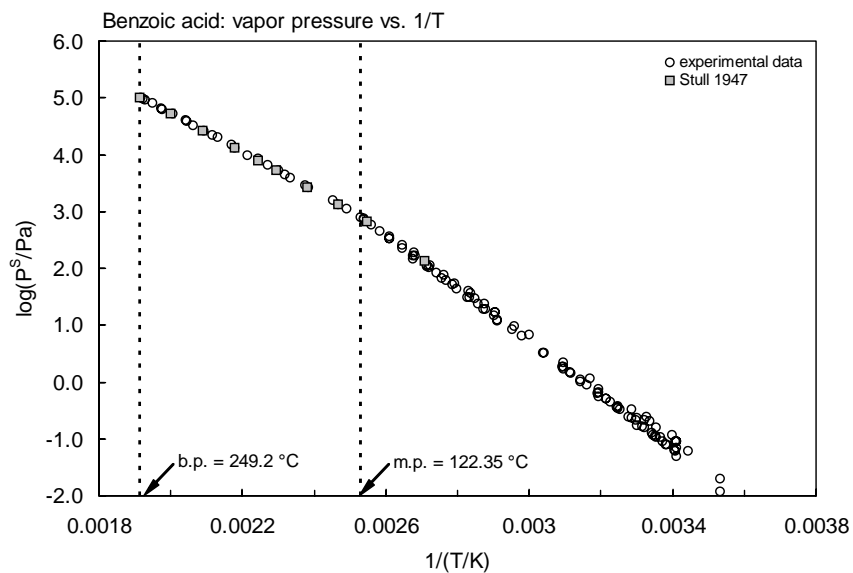
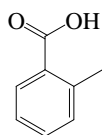


FIGURE 13.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for benzoic acid.

13.1.2.2 2-Methyl benzoic acid (*o*-Toluic acid)

Common Name: *o*-Toluic acid

Synonym: 2-methyl benzoic acid

Chemical Name: *o*-toluic acid, 2-methyl benzoic acid

CAS Registry No: 118-90-1

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

103.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

259 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.062 (115 $^{\circ}C$, Weast 1982–83; Verschueren 1983)

Molar Volume (cm^3/mol):

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.91 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)

3.91 (Weast 1982–83)

3.90 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.17 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

53.56 (Tsonopoulos & Prausnitz 1971)

53.5, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.170 (mp at $103.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

22300* (85.1 $^{\circ}C$, shake flask-residue volume, measured range 85.1–102.4 $^{\circ}C$, Sidgwick et al. 1915)

1185 (shake flask, Fühner 1924)

1162* (shake flask-weight titration, measured range 5–65 $^{\circ}C$, Strong et al. 1989)

1074* (shake flask-UV, Sugunan & Thomas 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log (P/mmHg) = -35.8816 - 3.2354 \times 10^3/(T/K) + 21.133 \cdot \log (T/K) - 3.0165 \times 10^{-2} \cdot (T/K) + 1.1587 \times 10^{-5} \cdot (T/K)^2$;
temp range 377–751 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.18 (shake flask-UV, Tomida et al. 1978)

2.81 (Scherrer & Howard 1979)

2.46 (shake flask at pH 1, Hansch & Leo 1987)

2.27 (shake flask-UV at pH 2, Da et al. 1992)

2.46 (recommended, Sangster 1993)

2.46 (recommended, pH 1, Hansch et al. 1995)

1.72 (RP-HPLC-RT correlation on short ODP column, pH 2, Donovan & Pescatore 2002)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 16 d (Alexander & Lustigman 1966; quoted, Verschueren 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.2.2.1

Reported aqueous solubilities of 2-methylbenzoic acid (o-toluic acid) at various temperatures

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993	
shake flask-residue volume		shake flask-titration		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
85.1	22300	5	568.3	20	825
109.1	36600	15	806.6	25	1074
118.3	50000	25	1162	35	1620
130.4	69900	35	1695	40	1883
143.7	102000	45	2522		
156.5	202300	55	3778		
160.2	314700	65	5775		
161.2	399200				
160.2	486300	$\Delta H_{sol}/(kJ\ mol^{-1}) = 28.92$			
154.6	601600	25°C			
147.4	701200				
119.8	846400				
97.2	905300				
93.7	918800				
94.4	938300				
96.0	959500				
102.4	1000000				
critical solution temp 161.2°C					
triple point 93.5°C					
mp 102.4°C					

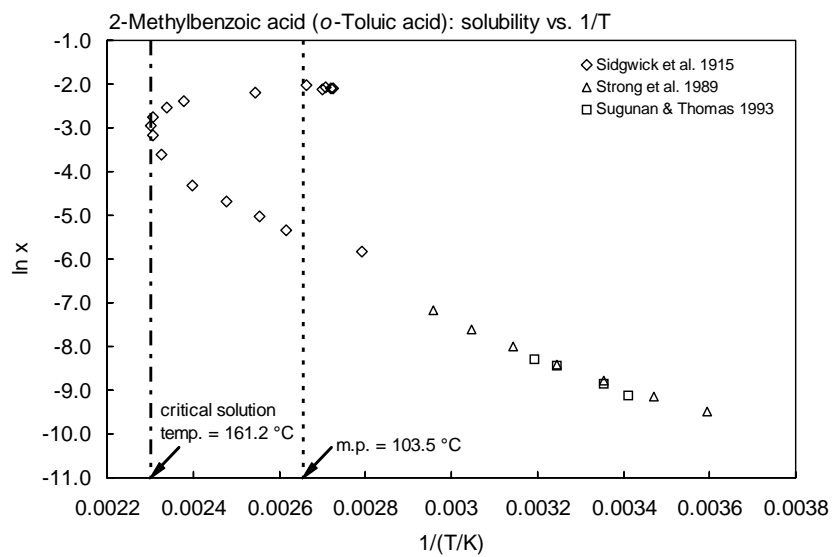
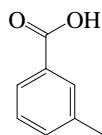


FIGURE 13.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-methylbenzoic acid.

13.1.2.3 3-Methyl benzoic acid (*m*-Toluic acid)

Common Name: *m*-Toluic acid

Synonym: 3-methyl benzoic acid

Chemical Name: *m*-toluic acid, 3-methyl benzoic acid

CAS Registry No: 99-04-7

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

109.9 (Lide 2003)

Boiling Point ($^{\circ}C$):

263.0 (sublimation, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

1.054 ($112^{\circ}C$, Weast 1982–83; Verschueren 1983)

Molar Volume (cm^3/mol):

129.2 ($112^{\circ}C$, Stephenson & Malanowski 1987)

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.270 (Weast 1982–83)

4.269 (Dean 1985)

4.220 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.73 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

10.96 (Tsonopoulos & Prausnitz 1971)

41.17, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.147 (mp at $109.9^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11600* ($80^{\circ}C$, shake flask-residue volume, measured range 80 – $110.5^{\circ}C$, Sidgwick et al. 1915)

982 (shake flask-residue volume method, Fühner 1924)

1700 (20 – $25^{\circ}C$, shake flask-GC, Urano et al. 1982)

872* (shake flask-weight titration, measured range 5 – $65^{\circ}C$, Strong et al. 1989)

1246* (shake flask-UV, Sugunan & Thomas 1993)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log(P_L/kPa) = 8.1472 - 3280.8/(T/K)$, temp range 473 – $533\ K$ (Antoine eq., liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.37 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)

2.43 (HPLC- k' correlation, Miyake & Terada 1982)

2.41 (shake flask-AS, Miyake et al. 1987)

2.39 (centrifugal partition chromatography CPC, Terada et al. 1987)

2.44; 2.47 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)

2.38 (shake flask-UV at pH 2, Da et al. 1992)

- 2.37 (recommended, Sangster 1993)
 2.37 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.2.3.1

Reported aqueous solubilities of 3-methylbenzoic acid (*m*-toluic acid) at various temperatures

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993	
shake flask-residue volume		shake flask-titration		shake flask-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
80	11600	5	449.3	20	1070
89.8	15300	15	621	25	1246
118.6	31300	25	872	35	1544
140.5	58800	35	1270	40	1720
153.3	99600	45	1852		
162.2	299400	55	2754		
162.1	401100	65	4115		
160.7	501000	75	6492		
157.7	601500				
145.1	711700	$\Delta H_{sol}/(\text{kJ mol}^{-1}) = 26.15$			
129.6	795700				
121.8	820600				
105.9	866700				
96.4	893200				
94.2	924500				
101.9	969300				
110.5	1000000				
critical solution temp 162.2°C					
triple point		142.0°C			
mp		110.5°C			

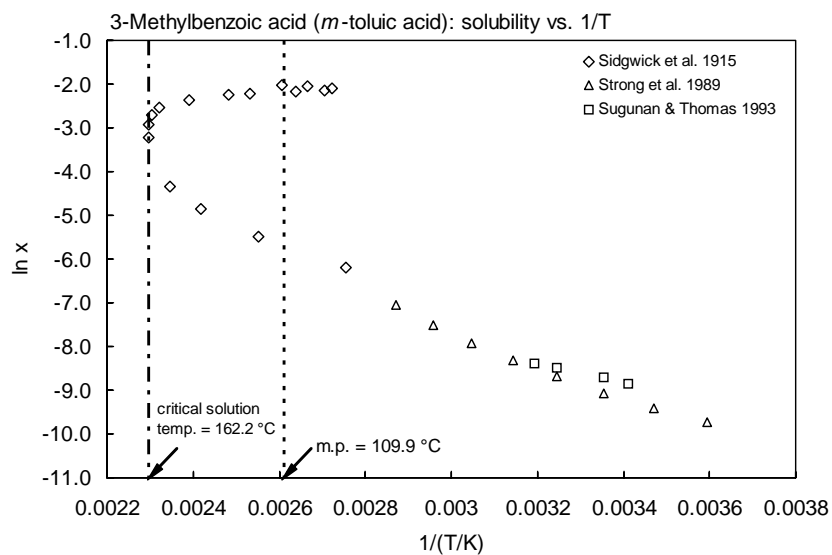
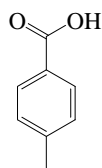


FIGURE 13.1.2.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-methylbenzoic acid (*m*-toluic acid).

13.1.2.4 4-Methyl benzoic acid (*p*-Toluic acid)

Common Name: *p*-Toluic acid

Synonym: 4-methyl benzoic acid

Chemical Name: *p*-toluic acid, 4-methyl benzoic acid

CAS Registry No: 99-94-5

Molecular Formula: $C_8H_8O_2$, $CH_3C_6H_4COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

179.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

275.0 (sublimation, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.37, 4.30 ± 0.09 (quoted, HPLC, Unger et al. 1978)

4.37, 4.41 ± 0.01 (quoted, HPLC, Unger et al. 1978)

4.36 (Weast 1982–83)

4.37, 4.26 (quoted, shake flask-TN, Clarke 1984)

4.362 (Dean 1985)

4.39 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.72 (Tsonopoulos & Prausnitz 1971)

23.81 (differential scanning calorimetry, Li et al. 2001)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

50.21 (Tsonopoulos & Prausnitz 1971)

50.21, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0304 (mp at $179.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11600* (100, shake flask-residue volume, measured range 100 – $176.8^{\circ}C$, Sidgwick et al. 1915)

383 (selected, Tsonopoulos & Prausnitz 1971)

343* (shake flask-weight titration, measured range 5 – $65^{\circ}C$, Strong et al. 1989)

331* (shake flask-UV, Sugunan & Thomas 1993)

378.5* (shake flask-titration, measured range 278.15 – $343.15 K$, Apelblat & Manzurola 1999)

$\ln [m/(mol kg^{-1})] = -264.605 - 9059.53/(T/K) + 40.069 \cdot \ln (T/K)$; temp range 278 – $343 K$ (shake flask-titration, Apelblat & Manzurola 1999)

371* (shake flask-laser monitoring observation technique, measured range 288.35 – $370.95 K$, Li et al. 2001)

393* ($26.4^{\circ}C$, synthetic method-laser technique, measured range 290.25 – $348.45 K$, Chen & Ma 2004)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

30.93* ($95.20^{\circ}C$, Knudsen effusion, measured range 95.2 – $134.96^{\circ}C$ (Davies & Jones 1954)

$\log (P/mmHg) = 128585 - 4968.7/(T/K)$; temp range 95.2 – $134.96^{\circ}C$ (Knudsen effusion, Davies & Jones 1954)

$\log (P/mmHg) = -67.6587 - 2.2339 \times 10^3/(T/K) + 33.347 \cdot \log (T/K) - 3.7709 \times 10^{-2} \cdot (T/K) + 1.313 \times 10^{-5} \cdot (T/K)^2$; temp range 453 – $773 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.27 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971)
- 2.22 \pm 0.02, 2.26 \pm 0.01 (HPLC-RT correlation, Unger et al. 1978)
- 2.36 (shake flask-UV at pH 2, Ezumi & Kubota 1980)
- 2.43 (calculated-HPLC- k' correlation, Miyake & Terada 1982)
- 2.34 (electrometric titration, Clarke 1984)
- 2.67 (HPLC-RT correlation, Garst 1984)
- 2.66 (centrifugal partition chromatography CPC, Terada et al. 1987)
- 2.38; 2.41 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)
- 2.35 (HPLC-RT correlation, Jenke et al. 1990)
- 2.26 (shake flask-UV at pH 2, Da et al. 1992)
- 2.34 (recommended, Sangster 1994)
- 2.27 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.15, 1.15, 1.30 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.77 (soil, quoted exptl., Meylan et al. 1992)
- 1.37 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

Environmental Fate Rate Constants or Half-Lives:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 8 d (Alexander & Lustigman 1966; quoted, Verschueren 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 13.1.2.4.1

Reported aqueous solubilities of 4-methylbenzoic acid (*p*-toluic) acid at various temperatures

1.

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993		Apelblat & Manzurola 1999	
shake flask-residue volume		shake flask-titration		shake flask-UV		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
100	11600	5	177.8	20	263	5.0	201.5
110	13600	15	243.5	25	331	11.0	249.2
114.4	15100	25	343	35	466	17.0	271.0
133.7	29600	35	486	40	534	21.5	309.1
141.4	49700	45	695			25.0	378.5
150.9	100800	55	1008			25.5	318.6
157.9	202700	65	1485			30.0	469.8
159.1	301400					30.0	488.8
158.5	405700	$\Delta H_{sol}/(kJ\ mol^{-1}) = 26.74$ 25°C				35.0	499.7
158.0	503800					35.0	501.1
152.6	605500					35.0	502.4
145.1	796800					40.0	593.7

TABLE 13.1.2.4.1 (Continued)

Sidgwick et al. 1915		Strong et al. 1989		Sugunan & Thomas 1993		Apelblat & Manzurola 1999	
shake flask-residue volume		shake flask-titration		shake flask-UV		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
156.5	925200					40.0	595.0
176.8	1000000					40.0	638.6
						45.0	721.7
Critical solution temp	159.1°C					50.0	887.8
Triple point	142°C					52.0	912.3
mp	176.8°C					55.0	1062
						58.0	1185
						60.0	1283
						61.0	1389
						65.0	1525
						67.0	1702
						70.0	1865
							$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 24.0$
							at 298.15 K
							$\ln S = A + B/T + C \ln T$
							S mol·kg ⁻¹
							A -264.605
							B 9059.53
							C 40.069

2.

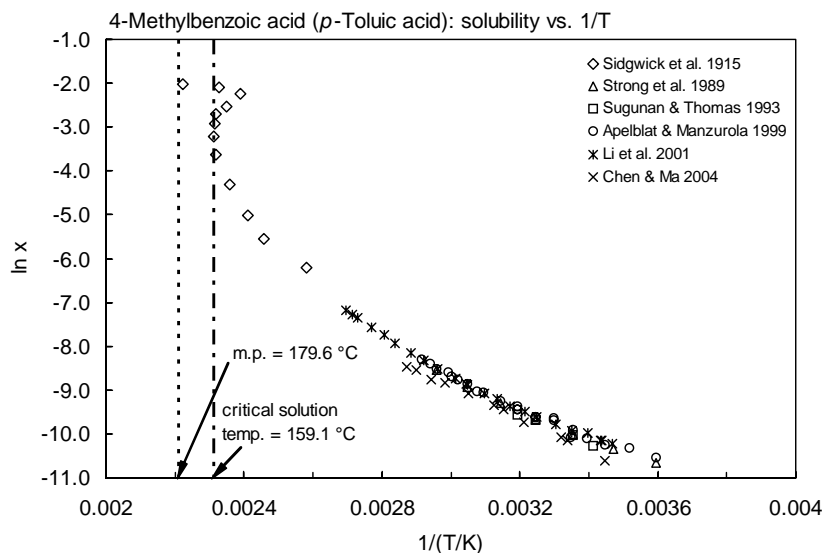
Li et al. 2001		Chen & Ma 2004	
shake flask-laser monitor		synthetic method	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
15.2	272.3	290.25	185.0
17.8	295	299.55	292.7
17.9	295	301.25	315.3
21.3	347.6	311.25	448.6
25.2	370.7	317.25	596.4
29.4	423.6	320.05	657.0
34.7	506.8	327.75	857.8
37.8	567.3	335.35	1109
42.1	650.5	339.85	1190
46.0	756.4	344.95	1465
49.8	869.9	348.35	1570
55.1	1051		
55.3	1074		
58.6	1210		
64.4	1520		
69.1	1838		
73.7	2201		
79.1	2723		
83.3	3260		
87.7	3911		

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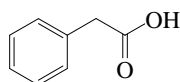
TABLE 13.1.2.4.1 (Continued)

Li et al. 2001		Chen & Ma 2004	
shake flask-laser monitor		synthetic method	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
93.1	4834		
95.5	5204		
97.8	5726		

$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 23.81$

FIGURE 13.1.2.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-methylbenzoic acid (*p*-toluic acid).

13.1.2.5 Phenylacetic acid



Common Name: Phenylacetic acid

Synonym: phenylethanoic acid, α -toluic acid, benzenecetic acid

Chemical Name: phenylacetic acid

CAS Registry No: 103-82-2

Molecular Formula: $C_8H_8O_2$, $C_6H_5CH_2COOH$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

76.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

265.5 (Stull 1947; Weast 1982–83; Dean 1985; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.081 (Verschuereen 1983)

Molar Volume (cm^3/mol):

124.8 ($77^{\circ}C$, Stephenson & Malanowski 1987)

157.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

4.28 ($18^{\circ}C$, Weast 1982–83)

4.31 (Sangster 1989)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.11 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

48.95 (Tsonopoulos & Prausnitz 1971)

41.42, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.312 (mp at $76.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

17700* (thermostatic and synthetic methods, measured range 25 – $86.7^{\circ}C$, Morrison 1944)

16600 ($20^{\circ}C$, Hodgman 1952)

17790 (selected, Tsonopoulos & Prausnitz 1971)

16600 ($20^{\circ}C$, quoted, Verschuereen 1983)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.835 (extrapolated-regression of tabulated data, temp range 97 – $265^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 15568.7/(T/K)] + 9.206178$; temp range 97 – $265.5^{\circ}C$ (Antoine eq., Weast 1972–73)

0.827 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.00148 - 3144.95/(-14.408 + T/K)$; temp range 370 – $539 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0056 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.41 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971)

1.41 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

1.51 (shake flask-UV, Yaguzhinskii et al. 1973)

1.94 (RP-LC-RT correlation, Hanai & Hubert 1982)

1.45 (shake flask-UV at pH 3.5, Kuchar et al. 1982)

1.95 ± 0.04 ; 1.51 (exptl.-ALPM, selected best lit. value, Garst 1984)

1.41 (recommended, Sangster 1989, 1993)

1.34 ± 0.14, 1.07 ± 0.49 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC-k' correlation, Cichna et al. 1995)

1.41 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

1.49, 1.42, 1.45 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)

1.45 (soil, quoted exptl., Meylan et al. 1992)

1.42 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

1.45 (soil, quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 13.1.2.5.1

Reported aqueous solubilities of phenylacetic acid at various temperatures:

Morrison 1944

thermostatic and synthetic

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
25.0	17700
35.0	26005
45.0	39484
41.5	39211
58.4	49695
68.8	59225
76.5	69845
83.0	83188
86.7	93399

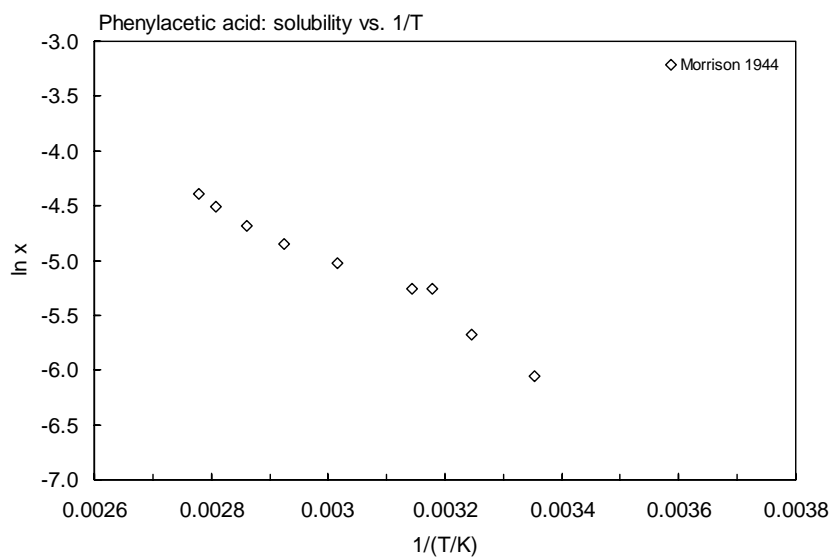
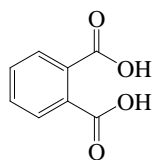


FIGURE 13.1.2.5.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phenylacetic acid.

13.1.2.6 Phthalic acid



Common Name: Phthalic acid

Synonym: 1,2-benzene dicarboxylic acid, *o*-phthalic acid

Chemical Name: 1,2-benzene dicarboxylic acid, *o*-phthalic acid

CAS Registry No: 88-99-3

Molecular Formula: $C_8H_6O_4$, $C_6H_4-1,2-(COOH)_2$

Molecular Weight: 166.132

Melting Point ($^{\circ}C$):

230 (dec., Lide 2003)

Boiling Point ($^{\circ}C$):

dec (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.593 (Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

173.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.89, 5.51 (pK_1 , pK_2 , Weast 1982–83)

2.95, 5.408 (pK_1 , pK_2 , Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section)

7014* (shake flask-synthetic method, measured range 25 – $85^{\circ}C$, McMaster et al. 1921):

7160* ($25.8^{\circ}C$, shake flask-synthetic method, measured range 25.8 – $113.8^{\circ}C$, Ward & Cooper 1930)

5400 ($14^{\circ}C$, Verschueren 1983)

6300 (Dean 1985)

7024* (shake flask, measured range 283.65 – 338.15 K, Apelblat & Manzurolo 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

$\log(P/mmHg) = -90.3221 - 3.2214 \times 10^3/(T/K) + 44.109 \cdot \log(T/K) - 5.0056 \times 10^{-2} \cdot (T/K) + 1.6895 \times 10^{-5} \cdot (T/K)^2$;
temp range 464 – 800 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m^3/mol):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.79 (shake flask-UV, Tomida et al. 1978)

0.15 (electrometric titration, Freese et al. 1979)

0.73 (shake flask at pH 1, Log P Database, Hansch & Leo 1987)

0.71 ($30^{\circ}C$, shake flask-UV at pH 1, Patrunkey & Pflegel 1992)

0.73 (recommended, Sangster 1993)

0.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

0.301, 1.49, 0.301	(sediment, Podzol soil, Alfidol soil, von Oepen et al. 1991)
1.07	(soil, quoted exptl., Meylan et al. 1992)
1.87	(soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
1.07	(soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation $78.4 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 2 \text{ d}$ in initial phase, $t_{1/2} = 15 \text{ d}$ in late phase in sludge -amended soil (Roslev et al. 1998)

Biota:

TABLE 13.1.2.6.1

Reported aqueous solubilities of *o*-phthalic acid at various temperatures

McMaster et al. 1921		Ward & Cooper 1930		Apelblat & Manzurola 1989	
shake flask-synthetic method		shake flask-synthetic method		shake flask-titration	
$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	T/K	$\text{S/g}\cdot\text{m}^{-3}$
25	7014	25.8	7160	283.65	2617
35	10125	43.7	13210	296.15	6546
45	14460	48.9	16470	298.15	7026
55	21680	58.0	22760	302.65	8633
65	32460	63.7	28970	307.15	9839
75	49260	77.8	53220	309.15	11020
85	78870	85.7	75940	311.15	11638
		94.8	118500	315.15	13936
		101.1	157900	317.15	15146
		113.8	294600	318.15	15164
				319.15	16705
				323.15	18893
				323.15	20554
				327.15	22926
				334.15	29783
				338.15	36955
$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 29.0$					

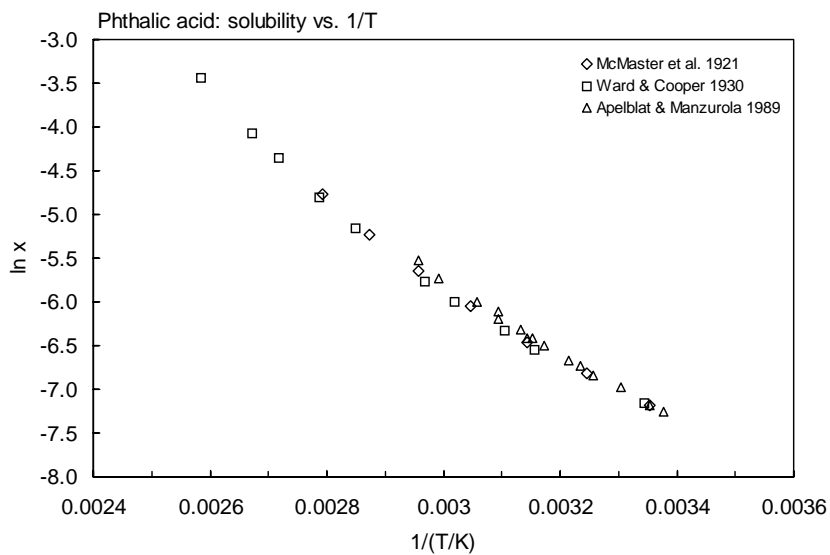
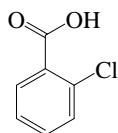


FIGURE 13.1.2.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phthalic acid.

13.1.2.7 2-Chlorobenzoic acid



Common Name: 2-Chlorobenzoic acid

Synonym: *o*-chlorobenzoic acid

Chemical Name: 2-chlorobenzoic acid, *o*-chlorobenzoic acid

CAS Registry No: 118-91-2

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

140.2 (Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Verschuereen 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5440 (Weast 1982–83, Verschuereen 1983)

1.5440 ($25^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

101.4 ($20^{\circ}C$, calculated-density)

155.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.920 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968; Weast 1982–83)

2.877 (Dean 1985)

3.850 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

25.73 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

62.34 (Tsonopoulos & Prausnitz 1971)

62.26, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0741 (mp at $140.2^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2130 (Osol & Kilpatrick 1933)

2114 (selected, Tsonopoulos & Prausnitz 1971)

2100 (Verschuereen 1983)

1100 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

$\log (P/mmHg) = -42.9847 - 3.1867 \times 10^3/(T/K) + 23.694 \cdot \log (T/K) - 3.0284 \times 10^{-2} \cdot (T/K) + 1.0828 \times 10^{-5} \cdot (T/K)^2$;
temp range 415–792 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.98 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1979, 1987)

2.63; 2.56 (calculated-fragment const., calculated- π const. Rekker 1977)

2.66 (shake flask-UV, Tomida et al. 1978)

1.99 (centrifugal partition chromatography, Berthod et al. 1988)

2.02 (shake flask-UV at pH 2, Da et al. 1992)

1.99 (recommended, Sangster 1993)

2.05 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: decomposition by soil microflora: $t_{1/2} > 64$ d, biodegradation by waste water at pH 7.3 and 30°C, $t_{1/2} > 25$ d, and degradation by soil suspension at pH 7.3 and 30°C; $t_{1/2} = 7$ –14 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);
complete degradation of 16 mg/L by soil in 7–14 d (Haller 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

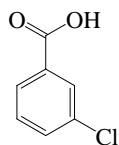
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.8 3-Chlorobenzoic acid



Common Name: 3-Chlorobenzoic acid

Synonym: *m*-chlorobenzoic acid

Chemical Name: 3-chlorobenzoic acid, *m*-chlorobenzoic acid

CAS Registry No: 535-80-8

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

158 (Weast 1982–83; Verschueren 1983; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Verschueren 1983; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.4960 ($25^{\circ}C$, Weast 1982–83; Verschueren 1983; Dean 1985)

Molar Volume (cm^3/mol):

104.7 ($25^{\circ}C$, calculated-density)

155.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.82 (Weast 1982–83)

3.83 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.85 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

55.65 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.0496$ (mp at $158^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

385 (Osol & Kilpatrick 1933)

398 (selected, Tsonopoulos & Prausnitz 1971)

400 ($0^{\circ}C$, Verschueren 1983)

400 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.68 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979)

2.65, 2.52 (calculated-fragment const., calculated- π const, Rekker 1977)

0.89 (HPLC-RT correlation, Veith et al. 1979)

2.57 (HPLC- k' correlation, Miyake & Terada 1982)

2.62 (centrifugal partition chromatography, Terada et al. 1987)

2.51; 2.58 (shake flask at pH 1; HPLC-RT correlation, Wang et al. 1989)

2.72 (shake flask-UV at pH 2, Da et al. 1992)

2.60 (recommended, Sangster 1993)

2.68 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct aqueous photolysis $k = 0.013 \pm 0.001 \text{ min}^{-1}$ with $t_{1/2} = 55 \text{ min}$ (Stegeman et al. 1993).

Oxidation:

Hydrolysis:

Biodegradation: decomposed by soil microflora, $t_{1/2} = 32 \text{ d}$ (Alexander & Lustigman 1966; quoted, Verschueren 1983);

complete degradation of 16 mg/L by soil and by wastewater in 7–14 d (Haller 1978).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

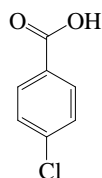
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.9 4-Chlorobenzoic acid



Common Name: 4-Chlorobenzoic acid

Synonym: *p*-chlorobenzoic acid

Chemical Name: 4-chlorobenzoic acid, *p*-chlorobenzoic acid

CAS Registry No: 74-11-3

Molecular Formula: $C_7H_5ClO_2$, ClC_6H_4COOH

Molecular Weight: 156.567

Melting Point ($^{\circ}C$):

243.0 (Weast 1982–83; Verschueren 1983; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Verschueren 1983)

Density (g/cm^3 at $20^{\circ}C$):

1.541 ($24^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

155.7 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.98 (McDaniel & Brown 1958; quoted, Pearce & Simkins 1968)

3.98 (Weast 1982–83)

3.98, 3.85 (quoted, shake flask-TN, Clarke 1984)

3.986 (Dean 1985)

3.850 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

32.26 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

62.76 (Tsonopoulos & Prausnitz 1971)

62.9, 56 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.00726$ (mp at $243^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

68.0 (Osol & Kilpatrick 1933)

72.6 (selected, Tsonopoulos & Prausnitz 1971)

77.0 (Verschueren 1983)

200 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.65 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)

2.65; 2.52 (calculated-fragment const., calculated- π const., Rekker 1977)

2.53; 2.65 (HPLC- k' correlation, Miyake & Terada 1982)

2.66 (electrometric titration, Clarke 1984)

2.72 (shake flask-OECD 1981 Guidelines., Geyer et al. 1984)

2.65 (centrifugal partition chromatography, Terada et al. 1987)

2.60; 2.67 (shake flask at pH 1, HPLC-RT correlation, Wang et al. 1989)

2.67 (HPLC-RT correlation, Wang et al. 1989)

- 2.65 (HPLC-RT correlation, Hayward et al. 1990)
- 2.71 (countercurrent chromatography, average value, Vallat et al. 1990)
- 2.66 (centrifugal partition chromatography; El Tayar et al. 1991)
- 2.62 (shake flask-UV at pH 2, Da et al. 1992)
- 2.65 (recommended, Sangster 1994)
- 2.65 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- < 1.0, 1.80, 2.23 (golden orfe, algae, activated sludge, Freitag et al. 1982)
- 1.80, 1.99 (alga *chlorella fusca*, wet wt. basis, calculated- K_{OW} , Geyer et al. 1984)
- < 1.0, 1.78, 2.23 (golden ide, algae, activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

$k(aq.) \leq 0.15 \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2–6 and $22 \pm 1^\circ\text{C}$, with $t_{1/2} \geq 3 \text{ d}$ at pH 7 (Yao & Haag 1991).

Hydrolysis:

Biodegradation: decomposition by a soil microflora, $t_{1/2} = 64 \text{ d}$; degradation by waste water or soil suspension at pH 7.3 and 30°C , $t_{1/2} > 25 \text{ d}$ (quoted, Verschueren 1983).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} \geq 3 \text{ d}$ at pH 7 based on reaction rate with ozone in water (Yao & Haag 1991)

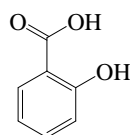
Groundwater:

Sediment:

Soil:

Biota:

13.1.2.10 Salicylic acid



Common Name: Salicylic acid

Synonym: 2-hydroxybenzoic acid, *o*-hydroxybenzoic acid

Chemical Name: salicylic acid, 2-hydroxybenzoic acid

CAS Registry No: 69-72-7

Molecular Formula: $C_7H_6O_3$, HOC_6H_4COOH

Molecular Weight: 138.121

Melting Point ($^{\circ}C$):

159.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

256 (Verschuereen 1983)

Density (g/cm^3 at $20^{\circ}C$):

1.443 (Weast 1982–83; Verschuereen 1983)

Molar Volume (cm^3/mol):

95.7 ($20^{\circ}C$, calculated-density)

147.4 ($158.6^{\circ}C$, Stephenson & Malanowski 1987)

142.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

3.009 (Korman & La Mer 1936)

3.52 ± 0.03 (HPLC, Unger et al. 1978)

3.29 ± 0.03 (HPLC, Unger et al. 1978)

2.96 (equilibrium titration, Clarke & Cahoon 1987)

2.97 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.0484 (mp at $159^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5570* ($50^{\circ}C$, synthetic method, measured range 50 – $159^{\circ}C$, critical solution temp. $89.5^{\circ}C$, Sidgwick & Ewbank 1921)

1840* ($20^{\circ}C$, synthetic method, measured, range 10 – $87^{\circ}C$, Bailey 1925)

1800 ($20^{\circ}C$, Hodgman 1952; Verschuereen 1983)

1550 (shake flask-UV, Yalkowsky et al. 1983)

2555* (shake flask-TN, measured range 283.15 – $339.15 K$, Apelblat & Manzurola 1989)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($113.7^{\circ}C$, summary of literature data, temp range 113.7 – $159^{\circ}C$, Stull 1947)

30.93* ($95.20^{\circ}C$, transpiration method, measured range 95.2 – $134.96^{\circ}C$, Davies & Jones 1954)

$\log (P/mmHg) = 12.8585 - 4968.7/(T/K)$, temp range 70.48 – $114.11^{\circ}C$ (transpiration, Davies & Jones 1954)

$\log (P/mmHg) = [-0.2185 \times 18920.7/(T/K)] + 10.822961$; temp range 113.7 – $256.0^{\circ}C$ (Antoine eq., Weast 1972–73)

2.85 ($70.5^{\circ}C$, effusion method, DePablo 1976)

0.0208 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.9834 - 4968.7/(T/K)$; temp range 368 – $408 K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.53812 - 1049.95/(-228.144 + T/K)$; temp range 445 – $504 K$ (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 177.3858 - 1.2871 \times 10^4/(T/K) - 56.301 \cdot \log (T/K) - 1.6667 \times 10^{-7} \cdot (T/K) + 1.1353 \times 10^{-5} \cdot (T/K)^2;$$

temp range 432–739 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.00144 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

- 2.26 (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1971)
- 2.21 (shake flask, unpublished result, Leo et al. 1971)
- 2.24 (shake flask, pH 2, Korenman 1975)
- 2.38 (shake flask-UV, Tomida et al. 1978)
- 2.00 ± 0.01 , 2.18 ± 0.01 (HPLC-RT correlation, Unger et al. 1978)
- 2.26, 2.21, 2.24, 2.25, 0.95 (quoted lit. values; Hansch & Leo 1979)
- 1.90 (HPLC-RT correlation, Butte et al. 1981)
- 2.25 ± 0.03 (exptl.-ALPM, Garst & Wilson 1984)
- 1.13, 1.92 (HPLC- k' correlation, Haky & Young 1984)
- 2.21 (shake flask-HPLC at pH 2, Bundgaard et al. 1986; Bundgaard & Nielsen 1988)
- 2.34 (electrometric titration, Clarke & Cahoon 1987)
- 2.24 (shake flask-radiochemical method, at pH 0.5, Laznicek et al. 1987)
- 1.08 (RP-TLC retention time correlation, Jack et al. 1988)
- 0.78 (shake flask-UV, Kuban 1991)
- 2.64 (centrifugal partition chromatography, Ilchmann et al. 1993)
- 2.26 (recommended, Sangster 1993)
- 2.11 (recommended, pH 7.4, Hansch et al. 1995)
- 1.70 (pH 7.0), -0.90 (pH 7.4); 2.26 (literature values; Hansch et al. 1995)
- 2.02 (shake flask-micro-volume liquid-liquid flow extraction system, Carlsson & Karlberg 2000)
- 1.44 (shake flask, buffered with 20 mM phosphate buffer pH 7.4, Carlsson & Karlberg 2000)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constants $k < 600 \text{ M}^{-1} \text{ s}^{-1}$ at pH 1.3–3, $k = (30 \pm 10) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ at pH 4–7 using 4 mM *t*-BuOH as scavenger for the reaction with ozone in water and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983a);

rate constants $k < 500 \text{ M}^{-1} \text{ s}^{-1}$ for protonated species, $k = (2.8 \pm 3) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species for the reaction with ozone in water using 4 mM *t*-BuOH as scavenger at pH 1.5–7 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983b).

Hydrolysis:

Biodegradation: decomposition by a soil microflora in 2 d (Alexander & Lustigman 1966; quoted, Verschuereen 1983);

average rate of biodegradation $95.0 \text{ mg COD g}^{-1} \cdot \text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Groundwater:

Sediment:

Soil:
Biota:

TABLE 13.1.2.10.1
Reported aqueous solubilities of salicylic acid at various temperatures

Sidgwick & Ewbank 1921		Bailey 1925		Apelblat & Manzurola 1989	
synthetic method		synthetic method		shake flask-titration	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
50.0	5570	10	1310	283.15	1533
56.0	7170	20	1840	298.15	2555
80.0	20260	30	2610	307.15	3385
97.9	52700	40	3950	317.15	4393
101.4	80200	50	5920	318.15	5196
105.6	168200	60	8640	320.15	5156
106.7	340200			323.15	5697
107.2	488180			324.15	6027
109.5	65400			325.15	6502
119.5	80000			327.15	7166
131.8	89750			328.15	7401
159.0	100000			330.65	8502
				334.65	10021
				339.15	11433
critical solution temp 89.5°C				$\Delta H_{\text{sol}}/(\text{kJ mol}^{-1}) = 24.0$ for temp range 288–313 K	

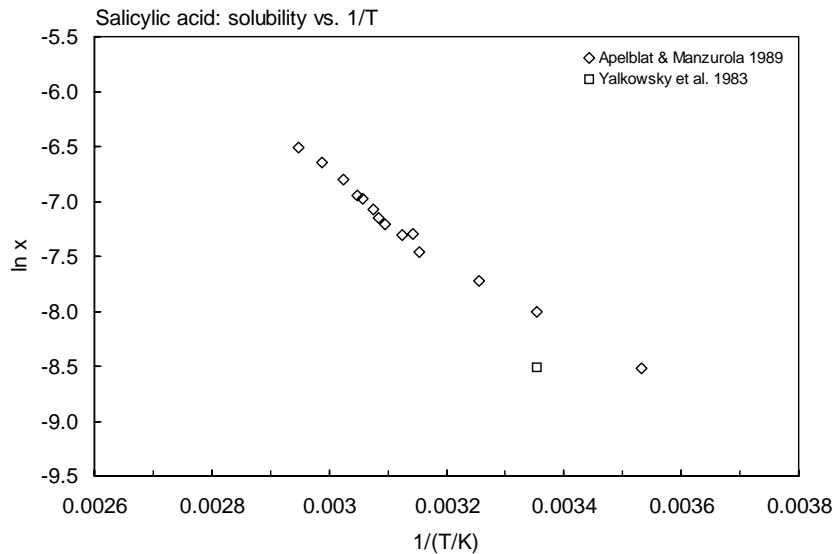


FIGURE 13.1.2.10.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for salicylic acid.

TABLE 13.1.2.10.2

Reported vapor pressures of salicylic acid at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log P = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log P = A - B/(C + T/K) \quad (3)$$

$$\log P = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Davies & Jones 1954	
summary of literature data		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa
113.7	133.3	95.20	30.93
136.0	666.6	100.49	48.66
146.2	1333	105.18	70.79
156.8	2666	109.96	103.7
172.2	5333	115.01	153.3
182.0	7999	119.98	220.4
193.4	13332	125.13	322.9
210.0	26664	134.96	649.3
230.5	53329		
256.0	101325	mp/°C	158.0–158.6
mp/°C	159	eq. 1	P/mmHg
		A	12.8585
		B	4968.7
$\Delta H_{\text{subl}}/(\text{kJ mol}^{-1}) = 95.144$			

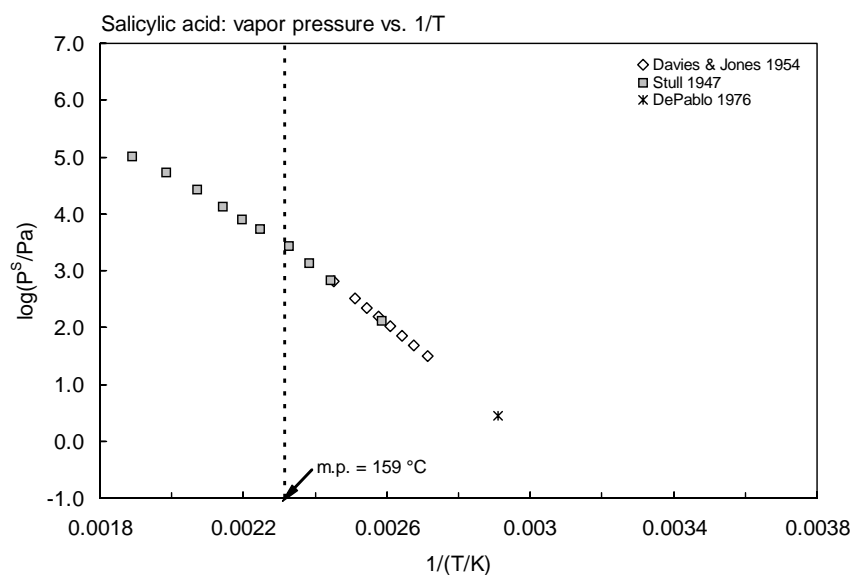
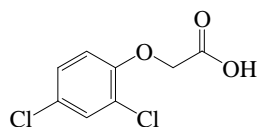


FIGURE 13.1.2.10.2 Logarithm of vapor pressure versus reciprocal temperature for salicylic acid.

13.1.2.11 2,4-Dichlorophenoxyacetic acid (2,4-D) (See also [Chapter 17](#), Herbicides)

Common Name: 2,4-Dichlorophenoxyacetic acid

Synonym: 2,4-D

Chemical Name: 2,4-dichlorophenoxyacetic acid

CAS Registry No: 94-75-7

Molecular Formula: $C_8H_6Cl_2O_3$, $Cl_2C_6H_3OCH_2COOH$

Molecular Weight: 221.038

Melting Point ($^{\circ}C$):

140.5 (Hartley & Kidd 1987; Howard 1991; Lide 2003)

Boiling Point ($^{\circ}C$):

160 (at 0.4 mmHg, Dean 1985; Howard 1991)

215 (Neely & Blau 1985)

Density (g/cm^3 at $30^{\circ}C$):

1.565 (Neely & Blau 1985)

Molar Volume (cm^3/mol):

206.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

2.77 (potentiometric, Nelson & Faust 1969)

2.87 (spectrophotometric, Cessna & Grover 1978)

2.80 (Reinert & Rogers 1984)

2.64–3.31 (Howard 1991)

2.80 (selected, Wauchope et al. 1992)

2.97 (Sangster 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.0736 (mp at $140.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

522 (shake flask-UV, Leopold et al. 1960)

725 (Bailey & White et al. 1965)

725, 400, 900, 550 (review, Günther et al. 1968)

890 (Hamaker 1975)

900 (Kenaga 1980a,b; Kenaga & Goring 1980)

600 ($20^{\circ}C$, Khan 1980)

470 (20 – $25^{\circ}C$, pH 5.6, Geyer et al. 1981)

633, 812 (15, $25^{\circ}C$, shake flask method, average values of 5 laboratories, OECD 1981)

620 ($20^{\circ}C$, Kidd & Hartley 1987; Worthing 1983)

609 (Gerstl & Helling 1987)

682 (Yalkowsky et al. 1987; quoted, Howard 1991)

703 (Gustafson 1989)

900, 600, 890, 703, 1072 (quoted, Wauchope et al. 1992)

890 (20 – $25^{\circ}C$, selected, Wauchope et al. 1992)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated):

8.0×10^{-5} (Hamaker 1975)

0.180–1.69 (transpiration method, Spencer 1976)

53.0 ($160^{\circ}C$, Kidd & Hartley 1983, 1987)

8.0×10^{-5} (recommended, Neely & Blau 1985; Lyman 1985)

1.00 ($20^{\circ}C$, selected, Suntio et al. 1988)

- 0.0032 (estimated from Henry's law constant, Howard 1991)
 5.6×10^{-5} (selected, Mackay & Stiver 1991)
 1.3×10^{-5} , 8.0×10^{-5} , 1.07×10^{-3} (quoted, Wauchope et al. 1992)
0.00107 (20–25°C, selected, Wauchope et al. 1992)

Henry's Law Constant (Pa·m³/mol):

- 0.55 (calculated-P/C, Suntio et al. 1988)
 1.03×10^{-3} (calculated-bond contribution, Howard 1991)

Octanol/Water Partition Coefficient, log K_{OW}:

- 2.81 (shake flask-AS, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1979; Hansch & Leo 1985)
2.59 (electrometric titration, Freese et al. 1979)
1.57 (Kenaga & Goring 1980, Kenaga 1980b)
1.57, 4.88 (shake flask-OECD 1981 Guidelines, Geyer et al. 1984)
−1.36 (Gerstl & Helling 1987)
2.65 (shake flask, Hansch & Leo 1987)
2.65 (centrifugal chromatography, Ilchmann et al. 1993)
2.81 (recommended, Sangster 1993)
2.81 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 1.11, −0.097 (calculated-S, K_{OW}, Kenaga 1980a)
−2.46, 1.30 (beef fat, fish, Kenaga 1980b)
0.778, 1.94 (alga *Chlorella fusca*: exptl. 24 h exposure, calculated-S, Geyer et al. 1981)
0.778, < 1.0, 1.23 (algae, golden orfe, activated sludge, Freitag et al. 1982)
0.00 (fish, microcosm conditions, Garten & Trabalka 1983)
0.778, 1.23 (algae, calculated-K_{OW}, Geyer et al. 1984)
1.11 (calculated, Isensee 1991)
−5.0 (bluegill sunfish and channel catfish, Howard 1991)
−2.70 (frog tadpoles, Howard 1991)
−3.0, −2.52 (pH 7.8, seaweeds, Howard 1991)
0.778, 0.85 (quoted: alga, fish, Howard 1991)

Sorption Partition Coefficient, log K_{OC}:

- 1.30, 2.0 (quoted, calculated, Kenaga 1980a)
1.30, 2.11 (quoted, Kenaga & Goring 1980)
1.68, 1.86, 1.68; 1.76 (commerce soil, Tracy soil, Catlin soil; average value of 3 soils, McCall et al. 1981)
2.25, 2.04, 2.35 (soil I-very strongly acid sandy soil pH 4.5–5.5, soil II-moderately or slightly acid loamy soil pH 5.6–6.5, soil III-slightly alkaline loamy soil pH 7.1–8.0, OECD 1981)
1.29 (soil, Neely & Blau 1985)
1.61 (soil, quoted, Sabljic 1987)
1.75, 2.00 (quoted, calculated-MCI χ , Gerstl & Helling 1987)
1.29–2.13 (soil, quoted values, Howard 1991)
1.30 (selected, Mackay & Stiver 1991)
1.00, 1.23, 2.29 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
1.30, 1.78, 1.51, 1.26, 1.72, 1.75, 1.76 (soil, quoted, Wauchope et al. 1992)
1.30 (soil, selected, Wauchope et al. 1992)
0.68 (calculated-K_{OW}, Kollig 1993)

Environmental Fate Rate Constants, k, or Half-Lives, t_{1/2}:

- Volatilization: volatilization from water is negligible, calculated volatilization t_{1/2} = 660 d from soil of 1 cm deep and t_{1/2} = 7.1 yr from 10 cm deep (Howard 1991).
Photolysis: aqueous photolysis t_{1/2} = 2–4 d when irradiated at 356 nm, t_{1/2} = 50 min in water when irradiated at 254 nm, and t_{1/2} = 29–43 d when exposed to September sunlight (Howard 1991).

Oxidation: photooxidation $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991).

Hydrolysis: no hydrolyzable groups and rate constant at neutral pH is zero (Kollig et al. 1987; selected, Howard et al. 1991); generally resistant to hydrolysis, may become important at $\text{pH} > 8$ (Howard 1991).

Biodegradation: degradation kinetics not first-order, time for 50% decomposition in six soils: $t_{1/2} = 5$ d in Commerce soil, $t_{1/2} = 1.5$ d in Catlin soil, $t_{1/2} = 3.9$ d in Keith soil, $t_{1/2} = 3.0$ d in Cecil soil, $t_{1/2} = 2.5$ d in Walla-Walla soil and $t_{1/2} = 8.5$ d in Fargo soil, with an average time of 4 d (McCall et al. 1981);

easily degraded under aerobic conditions with $t_{1/2} = 1.8$ and 3.1 d for cometabolism and metabolism respectively, under anaerobic conditions the degradation rate decreases and the $t_{1/2} = 69$ and 135 d (Liu et al. 1981; quoted, Muir 1991);

second-order $k = (3.6\text{--}28.8) \times 10^{-6}$ $\text{mL cell}^{-1} \text{d}^{-1}$ in natural water (Paris et al. 1981; quoted, Klečka 1985);

first-order $k < 0.14\text{--}0.07$ d^{-1} in river water at 25°C (Nesbitt & Watson 1980; quoted, Klečka 1985);

$k = 0.058 \pm 0.006$ d^{-1} in lake water at 29°C (Subba-Rao et al. 1982; quoted, Klečka 1985; quoted, Muir 1991);

$k = 0.08\text{--}0.46$ d^{-1} in soil at 25°C (McCall et al. 1981; quoted, Klečka 1985);

$t_{1/2}(\text{aq. aerobic}) = 240\text{--}1200$ h, based on unacclimated aerobic river die-away test data (Nesbitt & Watson 1980a, b; quoted, Howard et al. 1991; Muir 1991);

$t_{1/2}(\text{aq. anaerobic}) = 672\text{--}4320$ h, based on unacclimated aqueous screening test data (Liu et al. 1981; selected, Howard et al. 1991);

first-order $k = 0.035$ d^{-1} in die-away test, $k = 0.029$ d^{-1} in CO_2 evolution test in soil and $k = 6.9 \times 10^{-1}$ $\text{mL} \cdot (\text{g bacteria})^{-1} \cdot \text{d}^{-1}$ by activated sludge cultures (Scow 1982);

biodegradation $t_{1/2} = 18$ to > 50 d in clear river water and $t_{1/2} = 10$ to 25 d in muddy water with lag times of 6 to 12 d; degradation with a mixture of microorganisms from activated sludge, soil, and sediments lead to $t_{1/2} = 1.8\text{--}3.1$ d under aerobic conditions and $t_{1/2} = 69\text{--}135$ d under anaerobic conditions (Howard 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.8\text{--}18$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radicals in air (Howard et al. 1991);

photooxidation $t_{1/2} = 23.9$ h for reactions with hydroxyl radicals in air (Howard 1991).

Surface water: $t_{1/2} = 48\text{--}96$ h, based on reported photolysis half-lives for aqueous solution irradiated at UV wavelength of 356 nm (Howard et al. 1991);

degradation $t_{1/2} = 14$ d in sensitized, filtered and sterilized river water, based on sunlight photolysis test of $1 \mu\text{g mL}^{-1}$ in distilled water (Zepp et al. 1975; quoted, Cessna & Muir 1991);

typical biodegradation $t_{1/2} = 10$ to < 50 d with longer expected in oligotrophic waters, photolysis $t_{1/2} = 29\text{--}43$ d for water solutions irradiated at sunlight (Howard 1991).

Groundwater: $t_{1/2} = 480\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: $t_{1/2} < 1$ d for degradation in sediments and lake muds (Howard 1991).

Soil: $t_{1/2} = 240\text{--}1200$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

biodegradation $t_{1/2} < 1$ d to several weeks, $t_{1/2} = 3.9$ and 11.5 d in 2 moist soils and $t_{1/2} = 9.4$ to 254 d in the same soils under dry conditions (Howard 1991);

field $t_{1/2} = 2\text{--}16$ d, with a selected value of 10 d (Wauchope et al. 1992).

Biota: depuration $t_{1/2} = 13.8$ h in daphnids, $t_{1/2} = 1.32$ d in catfish (Ellgehausen et al. 1980).

13.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 13.2.1

Summary of physical properties of carboxylic acids

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm³/mol		pK _a
							MW/ρ at 20°C	Le Bas	
Aliphatics:									
Formic acid	64-18-6	HCOOH	46.026	8.3	101	1	37.91	46.2	3.75
Acetic acid	64-19-7	CH ₃ COOH	60.052	16.64	117.9	1	57.24	68.4	4.75
Propionic acid	79-09-4	C ₂ H ₅ COOH	74.079	−20.5	141.15	1	74.60	90.6	4.87
Butyric acid	107-92-6	C ₃ H ₇ COOH	88.106	−5.1	163.75	1	92.00	112.8	4.82
Isobutyric acid	79-31-2	(CH ₃) ₂ CHCOOH	88.106	−46	154.45	1	91.00	112.8	4.86
<i>n</i> -Valeric acid	109-52-4	C ₄ H ₉ COOH	102.132	−33.6	186.1	1	108.77	135.0	4.83
3-Methylbutanoic acid	503-74-2	C ₅ H ₁₀ O ₂	102.132	−29.3	176.5	1	109.70	135.0	4.777
Trimethylacetic acid	75-98-9	(CH ₃) ₃ CCOOH	102.132	35	164	0.798		135.0	4.81
Hexanoic acid (Caproic acid)	142-62-1	C ₅ H ₁₁ COOH	116.158	−3	205.2	1	125.79	157.2	4.87
Octanoic acid	124-07-2	C ₇ H ₁₅ COOH	144.212	16.5	239	1		201.6	4.85
Stearic acid	57-11-4	C ₁₇ H ₃₅ COOH	284.478	69.3	350 dec	0.368	302.38	423.6	4.5
Oleic acid	112-80-1	C ₁₈ H ₃₄ O ₂	282.462	13.4	360	1	316.13	416.2	
Acrylic acid (2-Propenoic acid)	79-10-7	CH ₂ =CHCOOH	72.063	12.5	141	1	68.56	83.2	4.255
2-Butenoic (<i>cis</i> -)	503-64-0	CH ₃ CH=CHCOOH	86.090	15	169	1	83.85	105.4	4.5
2-Butenoic (<i>trans</i> -)	107-93-7	CH ₃ CH=CHCOOH	86.090	71.5	184.7	0.350		105.4	
Vinylacetic acid	625-38-7	CH ₂ =CHCH ₂ COOH	86.090	−35	169	1	85.31	105.4	4.35
2-Methylpropenoic acid	79-41-4	C ₄ H ₆ O ₂	86.090	16	162.5	1	84.79	105.4	4.66
Chloroacetic acid	79-11-8	ClCH ₂ COOH	94.497	63	189.3	0.424	67.29	89.3	2.85
Dichloroacetic acid	79-43-6	Cl ₂ CHCOOH	128.942	13.5	194	1	82.48	110.2	1.26
Trichloroacetic acid	76-03-9	Cl ₃ CCOOH	163.387	59.2	196.5	0.462	100.86	131.1	0.7
Aromatics:									
Benzoic acid	65-85-0	C ₆ H ₅ COOH	122.122	122.35	249.2	0.111		134.8	4.19
2-Methylbenzoic acid	118-90-1	CH ₃ C ₆ H ₄ COOH	136.149	103.5	259	0.170		157.0	3.91
3-Methylbenzoic acid	99-04-7	CH ₃ C ₆ H ₄ COOH	136.149	109.9	263	0.147		157.0	4.27
4-Methylbenzoic acid	99-94-5	CH ₃ C ₆ H ₄ COOH	136.149	179.6	275	0.0304		157.0	4.39
Phenylacetic acid	103-82-2	C ₆ H ₅ CH ₂ COOH	136.149	76.5	265.5	0.312	125.95	157.0	4.31
Phthalic acid	88-99-3	C ₆ H ₄ -1,2-(COOH) ₂	166.132	230 dec	dec	0.00974	104.29	173.6	
2-Chlorobenzoic acid	118-91-2	ClC ₆ H ₄ COOH	156.567	140.2	sublim	0.0741	101.4	155.7	

3-Chlorobenzoic acid	535-80-8	ClC ₆ H ₄ COOH	156.567	158	sublim	0.0496		155.7	3.82
4-Chlorobenzoic acid	74-11-3	ClC ₆ H ₄ COOH	156.567	243		0.00726		155.7	3.85
Salicylic acid	69-72-7	HO C ₆ H ₄ COOH	138.121	159		0.0484	95.72	142.2	2.97
Phenoxyacetic acid	122-59-8	C ₆ H ₅ OCH ₂ COOH	152.148	98.5	285 dec	0.190		164.4	
2,4-Dichlorophenoxyacetic acid	94-75-7	Cl ₂ C ₆ H ₃ OCH ₂ COOH	221.038	140.5	215	0.0736		206.2	
2,4,5-Trichlorophenoxyacetic acid	93-76-5	Cl ₃ C ₆ H ₂ OCH ₂ COOH	255.483	153	dec	0.0555		227.1	

* Assuming $\Delta S_{\text{fus}} = 56 \text{ J/mol K}$.

TABLE 13.2.2
Summary of selected physical-chemical properties of carboxylic acids at 25°C

Compound	Selected properties						Henry's law constant H/(Pa·m ³ /mol)		
	Solubility			Vapor pressure		log K _{ow}	calcd P/C	exptl ^a	calcd ^b
	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)	P ^S /Pa	P _L /Pa				
Aliphatics:									
Formic acid	miscible			5750	5750	−0.54		0.01832	
Acetic acid	miscible			2079	2079	−0.31		0.01825	0.0285
Propionic acid	miscible			435	435	0.26		0.018	0.0431
Butyric acid	miscible			84	84	0.79		0.0222	0.0650
Isobutyric acid	22800	258.8	258.8	185	185	0.79	0.715	0.0897	
<i>n</i> -Valeric acid	24000	235.0	235.0	19	19	1.39	0.081	0.0478	0.099
3-Methylbutanoic acid	4100	40.14	40.14	25	25		0.623	0.0844	
Hexanoic acid	9580	82.47	82.47	5	5	1.92	0.0606	0.0768	0.149
Octanoic acid	79.8	0.553	0.553	3.72	3.72		6.723		0.338
Stearic acid	340	1.195	3.248		1.69 × 10 ^{−6}	8.23			
Oleic acid				0.00113	0.00113	7.64			
Acrylic acid	miscible			550	550	0.43			
2-Methylpropenoic acid	8900	103.4	103.4	100	100	0.93	0.9673		
Chloroacetic acid	miscible				18.5	0.22			
Dichloroacetic acid	miscible			35	35	0.92			
Trichloroacetic acid					11	1.33			
Aromatics:									
Benzoic acid	3400	27.84	250.8	0.11	0.991	1.89	3.95 × 10 ^{−3}		
2-Methylbenzoic acid	1074	7.888	46.40			2.46			
3-Methyl benzoic acid	1246	9.152	62.26	1.39	9.456	2.37	0.1512		
4-Methylbenzoic acid	331	2.431	79.97			2.34			
Phenylacetic acid	16600	121.9	390.8	0.83	2.660	1.41	6.81 × 10 ^{−3}		
Phthalic acid	7000	42.14	4326			0.73			
2-Chlorobenzoic acid	2100	13.41	181.0			1.99			
3-Chlorobenzoic acid	400	2.555	51.51			2.60			
4-Chlorobenzoic acid	70	0.4471	61.58			2.65			
Salicylic acid	2300	16.65	344.0	0.0208	0.440	2.20	1.25 × 10 ^{−3}		
Phenoxyacetic acid	12000	78.87	415.1			2.81			
2,4-D	890	4.026	54.71	8.0 × 10 ^{−5}	0.001	2.65	1.99 × 10 ^{−5}		
2,4,5-T	278	1.088	19.61						

^a Brimblecombe et al. 1992; ^b Hine & Mookerjee 1975.

TABLE 13.2.3

Suggested half-life classes for carboxylic acids in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aliphatics:				
Formic acid	4	3	4	5
Acetic acid	3	3	4	5
Butyric acid	3	3	4	5
Hexanoic acid (Caproic acid)	3	3	4	5
Stearic acid (Octadecanoic acid)	3	3	4	5
Acrylic acid (2-Propenoic acid)	2	3	4	5
Vinylacetic acid	2	3	4	5
Chloroacetic acid	5	4	5	6
Aromatics:				
Benzoic acid	3	3	4	5
2-Methylbenzoic acid (<i>o</i> -Toluic acid)	3	3	4	5
Phenylacetic acid	3	3	4	5
Phthalic acid	3	3	4	5
2-Chlorobenzoic acid	4	5	6	7
Salicylic acid	3	3	4	5
2,4-Dichlorophenoxyacetic acid (2,4-D)	2	3	5	6
2,4,5-Trichlorophenoxyacetic acid (2,4,5-T)	3	4	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	<10
2	17 (~1 d)	10–30
3	55 (~2 d)	30–100
4	170 (~1 week)	100–300
5	550 (~3 weeks)	300–1,000
6	1,700 (~2 months)	1,000–3,000
7	5,500 (~8 months)	3,000–10,000
8	17,000 (~2 y)	10,000–30,000
9	~5 y	>30,000

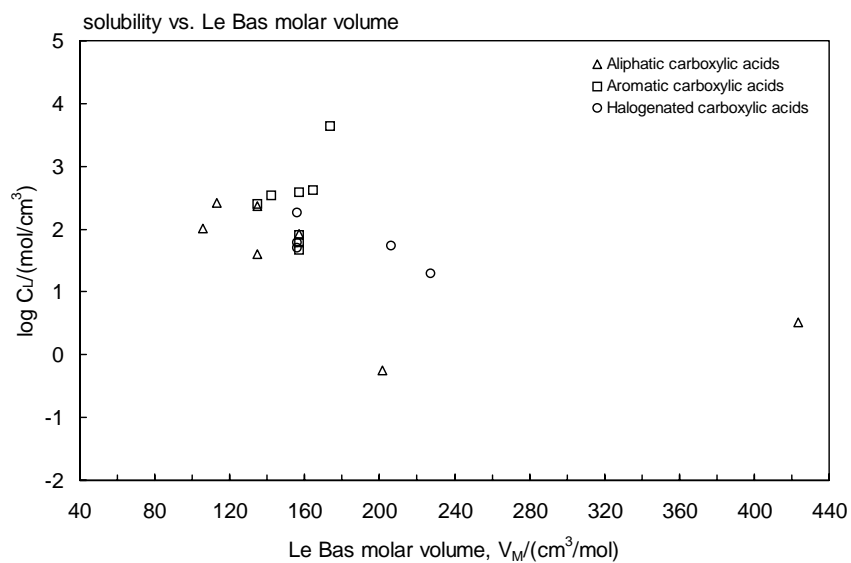


FIGURE 13.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.

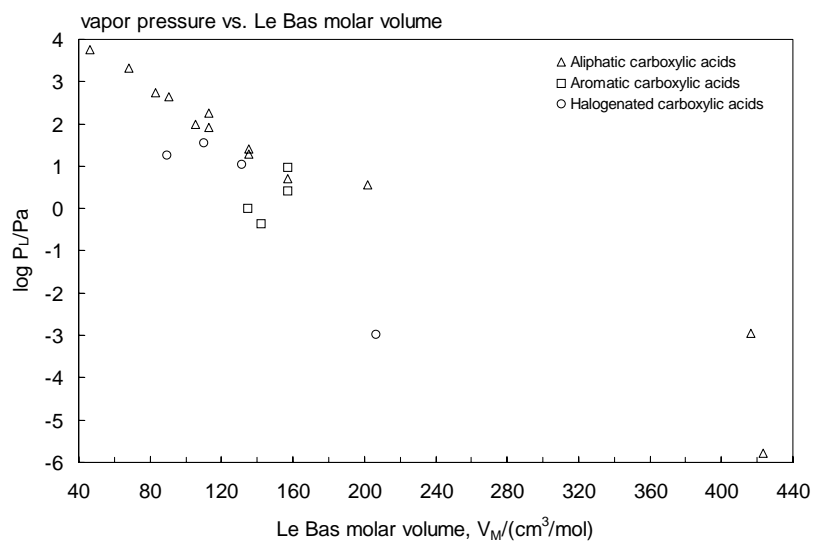


FIGURE 13.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for carboxylic acids.

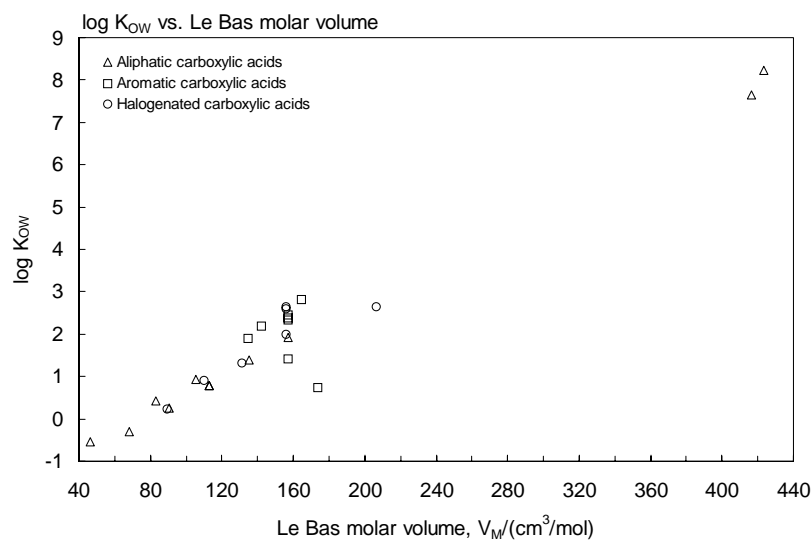


FIGURE 13.2.3 Octanol-water partition coefficient versus Le Bas molar volume for carboxylic acids.

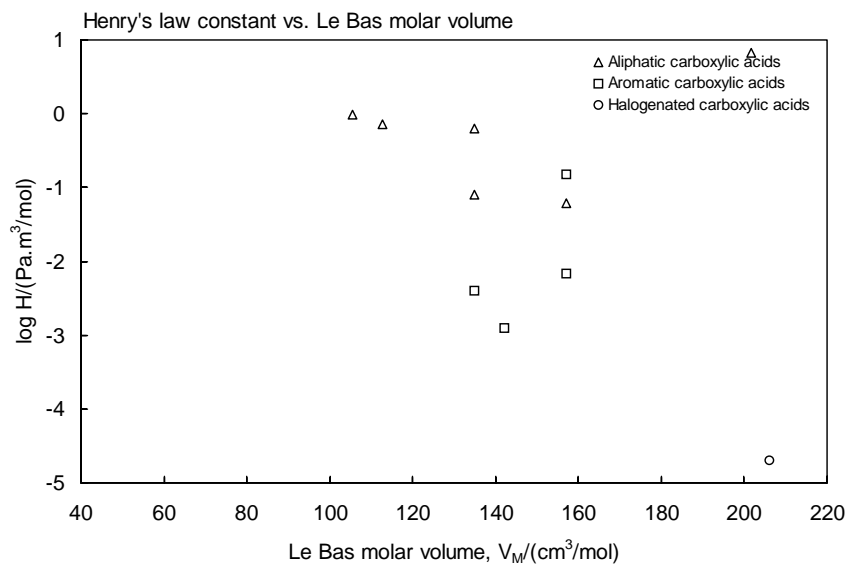


FIGURE 13.2.4 Henry's law constant versus Le Bas molar volume for carboxylic acids.

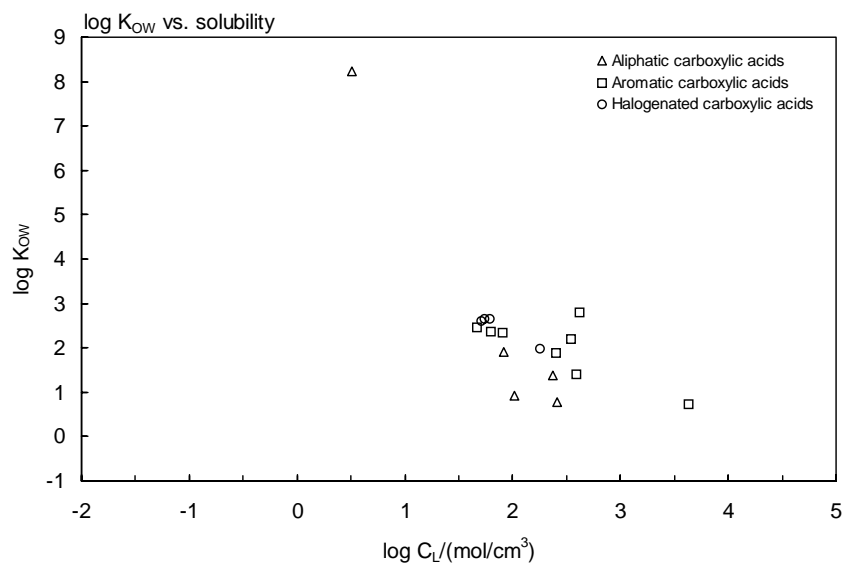


FIGURE 13.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for carboxylic acids.

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14 Phenolic Compounds

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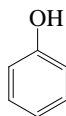
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14.1 LIST OF CHEMICALS AND DATA COMPILATIONS

14.1.1 ALKYLPHENOLS AND OTHER SUBSTITUTED PHENOLS

14.1.1.1 Phenol



Common Name: Phenol

Synonym: carbolic acid, phenic acid, phenylic acid, phenyl hydrate, phenyl hydroxide, hydroxybenzene, oxybenzene

Chemical Name: phenol

CAS Registry No: 108-95-2

Molecular Formula: C_6H_5OH

Molecular Weight: 94.111

Melting Point ($^{\circ}C$):

40.89 (Lide 2003)

Boiling Point ($^{\circ}C$):

181.87 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.5479 (supercooled liq., Ericksen & Dobbert 1955)

1.0576 (Weast 1982)

Acid Dissociation Constant, pK_a :

9.90 (Blackman et al. 1955, McLeese et al. 1979)

10.02 (Herington & Kynaston 1957; Callahan et al. 1979)

9.82 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)

10.0 (Serjeant & Dempsey 1979; Paris et al. 1982; Miyake et al. 1987; Tratnyek & Hoigné 1991)

9.92 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Varhaníčková et al. 1995)

10.05 (Saarikoski 1982; Saarikoski & Viluksela 1982)

9.90 (UV absorption, Hoigné & Bader 1983; Scully & Hoigné 1987)

9.99 (Dean 1985; Schultz & Cajina-Quezada 1987; Hersey et al. 1989)

10.93 (Miyake et al. 1987)

10.12 (UV spectrophotometry, Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

89.0 ($20^{\circ}C$, calculated-density)

103.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

56.13, 45.83 ($25^{\circ}C$, bp, Dreisbach 1955)

47.30 (at normal bp, Biddiscombe & Martin 1958)

45.689 (at normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

68.66 (at $25^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.514 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

36.63 (Tsonopoulos & Prausnitz 1971)

36.0, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.698 (mp at $40.89^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

86600* (synthetic method, measured range $20-65.86^{\circ}C$, Hill & Malisoff 1926)

83000 ($20^{\circ}C$, synthetic method, Jones 1929)

89300* ($22.7^{\circ}C$, thermostatic and synthetic methods, measured range $22.7-60.9^{\circ}C$, Morrison 1944)

- 88360 (shake flask-UV at pH 5.1, Blackman et al. 1955)
 79000* (20°C, synthetic method/shake flask-optical, measured range 0–68.3°C, Ericksen & Dobbert 1955)
 80000 (20°C, Mulley & Metcalf 1966)
 78000 (shake flask-spectrophotometry, Roberts et al. 1977)
 79750 (shake flask-GC, Kraij & Sincic 1980)
 76514 (generator column-HPLC, Wasik et al. 1981)
 150580 (20°C, shake flask-UV, Hashimoto et al. 1984)
 87000 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)
 84045* (shake flask-conductimetry, measured range 15.1–35°C, Achard et al. 1996)
 94100* (25.35°C, shake flask-optical method, measured range 298.5–336.7 K, Jaoui et al. 1999)
 83119* (23.15°C, shake flask-optical method, measured range 292.5–333.6 K, Jaoui et al. 2002)
 $\ln [S/(\text{mol kg}^{-1})] = 7.3013 - 853.62/(T/K)$; temp range 288–313 K (eq.-I derived using reported exptl. data, Jaoui et al. 2002)
 $\ln [S/(\text{mol kg}^{-1})] = 10.731 - 1931.7/(T/K)$; temp range 313–332 K (eq.-II derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 133.3* (44.8 °C, static method-manometer, measured range 44.8–181.4 °C, Kahlbaum 1898)
 28531* (141.1 °C, mercury manometer, measured range 141.1–181.1 °C, Goldblum et al. 1947)
 $\log (P/\text{mmHg}) = -2510/(T/K) + 8.395$; temp range: 141.1–181.1°C (Hg manometer, Goldblum et al. 1947)
 55.54* (extrapolated-regression of tabulated data, temp range 40.1–181.9°C, Stull 1947)
 7605* (107.15 °C, ebulliometry, measured range 107.15–181.75 °C, Dreisbach & Shrader 1949)
 1333* (70.50 °C, ebulliometry, measured range 70.50–181.7 °C, Vonterres et al. 1955)
 70.75 (calculated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 7.57893 - 1817.0/(205.0 + t/^{\circ}\text{C})$, temp range: 93–240°C, (Antoine eq. for liquid state, Dreisbach 1955)
 44.26* (24.85°C, gas saturation and diaphragm manometer measurements, measured range 0–37.5°C, Biddiscombe & Martin 1958)
 45.71 (gas saturation and diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
 $\log (P/\text{mmHg}) = 11.5638 - 3586.36/(t/^{\circ}\text{C} + 273)$; temp range 9–40°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P_L/\text{mmHg}) = 7.13457 - 1615.072/(t/^{\circ}\text{C} + 174.569)$; temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 45.07 (interpolated- Antoine eq., Andon et al. 1960)
 70.70 (20°C, supercooled liq., Andon et al. 1960)
 83.95 (extrapolated supercooled liquid value, Antoine eq., Weast 1972–73)
 $\log (P/\text{mmHg}) = [-0.2185 \times 11891.5/(T/K)] + 8.513843$; temp range 40.1–418.7°C (Antoine eq., Weast 1972–73)
 47.01 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.13301 - 1516.79/(174.954 + t/^{\circ}\text{C})$; temp range 107–182°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
 26.66, 133.3 (20°C, 40°C, Verschuereen 1977, 1983)
 16.27 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 454.610/(T/K)] \times 10^{\{1.00375 - 8.88757 \times 10^{-4} \cdot (T/K) + 6.83750 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 323.205–694.25 K, (Cox eq., Chao et al. 1983)
 46.91, 54.74 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.25543 - 1515.182/(174.182 + t/^{\circ}\text{C})$; temp range 107–181.75°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.70346 - 1793.899/(200.218 + t/^{\circ}\text{C})$; temp range 70.5–181.7°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 47.00 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.1330 - 1516.79/(174.95 + t/^{\circ}\text{C})$; temp range 107–182°C (Antoine eq., Dean 1985, 1992)
 55.00 (selected, Riddick et al. 1986)
 45.7, 45.32 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 10.6887 - 3586.36/(T/\text{K})$; temp range 282–313 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_S/\text{kPa}) = 10.71099 - 3594.703/(T/\text{K})$; temp range 273–313 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.25947 - 1516.072/(-98.581 + T/\text{K})$; temp range 383–473 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.34757 - 1482.82/(-113.862 + T/\text{K})$; temp range 455–655 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.57957 - 1710.287/(-80.273 + T/\text{K})$; temp range 314–395 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.26694 - 1522.07/(-97.834 + T/\text{K})$; temp range 387–456 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.30177 - 1548.368/(-94.612 + T/\text{K})$; temp range 449–526 K (Antoine eq.-VII, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.92874 - 2146.053/(-17.025 + T/\text{K})$; temp range 520–625 K (Antoine eq.-VIII, liquid, Stephenson & Malanowski 1987)

61.16 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)

$\log (P/\text{Pa}) = 37.91650 - 4155.615/(T/\text{K}) - 9.02308 \cdot \log (T/\text{K}) + 0.04526 \times 10^{-2} \cdot (T/\text{K})$; temp range: 394–455 K (four-parameter vapor pressure eq. using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)

$\log (P/\text{Pa}) = 127.08645 - 7292.585/(T/\text{K}) - 42.92601 \cdot \log (T/\text{K}) + 1.76834 \times 10^{-2} \cdot (T/\text{K})$; temp interval of investigation 380–455 K (four-parameter vapor pressure eq. derived using data of Dreisbach & Shrader 1949, Nesterova et al. 1990)

$\log (P/\text{mmHg}) = 23.5332 - 3.4961 \times 10^3/(T/\text{K}) - 4.899 \cdot \log (T/\text{K}) + 1.216 \times 10^{-4} \cdot (T/\text{K}) + 9.6537 \times 10^{-13} \cdot (T/\text{K})^2$; temp range 314–694 K (vapor pressure eq., Yaws 1994)

173* (40.09°C, ebulliometry, measured range 40–90°C, Tabai et al. 1997)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0402 (exptl., Hine & Mookerjee 1975; Howard 1989)

0.065, 1.082 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

0.0718* (27.0°C, gas stripping-GC, measured range –2.0 to 27.0°C Abd-El-Bary et al. 1986)

$k_H/\text{kPa} = 2.69 \times 10^9 \exp[-6120/(T/\text{K})]$, temp range –2 to 90°C (gas stripping-GC measurements plus reported data at higher temp., Abd-El-Bary et al. 1986)

1.245, 2.193, 3.322 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

0.0607* (extrapolated from temp dependence eq., Dohnal & Fenclová 1995)

$\ln K_{AW} = 8.701 - 5760/(T/\text{K})$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional literature data, Dohnal & Fenclová 1995)

0.0342* (313.24 K, derived from measured P, temp range 313.240–363.14 K, Tabai et al. 1997)

$k_H/\text{kPa} = 670.117 - 39274.5/(T/\text{K}) - 94.6679$; temp range 313–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

< 0.240 (gas stripping-GC, Altschuh et al. 1999)

0.0536 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

0.0320* (gas stripping-UV, measured range 284–302 K, Harrison et al. 2002)

$\ln [H/(M \text{ atm}^{-1})] = 5850/(T/\text{K}) - 11.6$; temp range 284–302 K, Harrison et al. 2002)

0.157* (dynamic equilibrium/gas stripping-GC/MS, measured range 5–25°C, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$. Additional data at other temperatures designated * are compiled at the end of this section:

1.46 (shake flask-UV, Fujita et al. 1964)

1.46 ± 0.01 (shake flask-UV, Iwasa et al. 1965)

1.42 (shake flask-UV at pH 7.4, Rogers & Cammarata 1969)

1.60 (shake flask, Kiezyk & Mackay 1971)

1.47 (Leo et al. 1971)

1.51 (shake flask-UV at pH 7.45, Umeyama et al. 1971)

1.49 (shake flask, Korenman 1972)

- 1.510* (20 °C, shake flask-concn ratio, measured range 10–60 °C, Korenman & Udalova 1974)
 1.46, 1.61 (LC- k' correlation, calculated- π const., Carlson et al. 1975)
 1.54 (shake flask-UV, Davis et al. 1976)
 1.45 (HPLC-RT correlation, Mirrlees et al. 1976)
 1.48 \pm 0.02 (shake flask at pH 7, Unger et al. 1978)
 1.48, 1.46, 1.49, 1.51, 0.62, 2.20 (literature values, Hansch & Leo 1979)
 1.46 (HPLC- k' correlation, Butte et al. 1981; Butte et al. 1987)
 1.45 (generator column-HPLC/UV, Wasik et al. 1981)
 1.54 (RP-HPLC- k' correlation, D'Amboise & Hanai 1982)
 1.28, 1.54 (RP-LC- k' correlation, calculated-fragment const. as per Rekker 1977, Hanai & Hubert 1982)
 1.54 (HPLC- k' correlation, Miyake & Terada 1982; Miyake et al. 1987)
 1.62 (inter-laboratory, shake flask average, Eadsforth & Moser 1983)
 1.16 (inter-laboratory, HPLC average, Eadsforth & Moser 1983)
 1.49, 1.53 \pm 0.09 (selected best lit. value, exptl.-ALPM, Garst 1984)
 1.46, 1.55 \pm 0.07 (selected best lit. value, exptl.-ALPM, Garst & Wilson 1984)
 1.08 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
 1.46 (RP-HPLC-RT correlation, Chin et al. 1986)
 1.00, 1.42 (HPLC- k' correlation, Eadsforth 1986)
 1.46 (shake flask-CPC centrifugal partition chromatography, Berthod et al. 1988)
 1.46 (RP-HPLC-capacity ratio correlation, Minick et al. 1988)
 1.46 (HPLC-RT correlation, Shigeota et al. 1988)
 1.52 \pm 0.01 (filter chamber-UV, Hersey et al. 1989)
 1.50 (recommended, Sangster 1989, 1993)
 1.52, 1.58, 1.69 (CPC-RV correlation, Gluck & Martin 1990)
 1.47 (shake flask-UV, Kramer & Henze 1990)
 1.37 \pm 0.06 (liquid-liquid extraction-flow injection-UV, Kubá 1991)
 1.57 (shake flask-GC, Kishino & Kobayashi 1994)
 1.46 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 4.16 (total ^{14}C in fathead minnow, mean exposure level 0.0025 $\mu\text{g}\cdot\text{mg}^{-1}$, Call et al. 1980)
 4.23 (total ^{14}C in fathead minnow, mean exposure level 0.0327 $\mu\text{g}\cdot\text{mg}^{-1}$, Call et al. 1980)
 4.20 (total ^{14}C in fathead minnow, mean value, Call et al. 1980)
 2.20 (goldfish, rate constant ratio k_1/k_2 , Nagel & Urich 1980)
 0.97 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 1.30, 2.30, 3.34 (golden ide, algae, activated sludge, Freitag et al. 1985)
 2.30 (*chlorella fusca*, Freitag et al. 1985; quoted, Howard 1989)
 1.20 (algae, maximum apparent BCF, Hardy et al. 1985)
 0.544 (algae, real BCF with biotransformation, Hardy et al. 1985)
 3.14 (*daphnia magna*, estimated- ^{14}C activity and on dry wt. basis, Dauble et al. 1986)
 2.44 (*daphnia magna*, based on elimination phase, Dauble et al. 1986)
 1.28 (*daphnia magna*, Dauble et al. 1986; quoted, Geyer et al. 1991)
 1.24 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, log K_{OC} :

- 1.43 (soil, Kenaga & Goring 1980)
 1.48 (20°C, sorption isotherm, converted form K_{OM} organic carbon in soils, Briggs 1981)
 1.15 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 1.57, 1.96 (silt loams, Scott et al. 1983, quoted, Howard 1989)
 3.46 (untreated fine sediment, Isaacson & Frink 1984)
 3.49 (untreated coarse sediment, Isaacson & Frink 1984)
 1.35 (HPLC- k' correlation, mobile phase buffered to pH 3, Hodson & Williams 1988)
 2.17 (soil, calculated- K_{OW} , Howard 1989)
 2.4, 2.43 (soil: quoted, calculated-MCI χ , Meylan et al. 1992)

- 2.68, 2.38 (natural zeolite modified with a cation surfactant HDTMA with surface coverage of 100, 200 mmol/kg at pH 7, shake flask-sorption isotherm, Li et al. 2000)
- 1.43 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 1.42, 1.00, 1.24 (RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
- 1.59, 1.67 (HP:LC- k' correlation, C_{18} column, Hong et al. 1996)
- 1.32; 2.43 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
- 1.56, 1.556, 1.255, 1.307, 1.52 (soil, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
- 1.310, 1.750, 1.281, 1.601, 1.544 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)
- 1.310, 1.750, 1.281, 1.601, 1.544 (soil, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
- 1.37, 1.34 (soils: organic carbon $OC \geq 0.1\%$ and pH 3.2–7.4, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 3.2$ months for evaporation from water (Howard 1989);

$t_{1/2} = 88$ d, calculated for evaporation from a model river of 1 m deep with a current of 3 m/s and with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: phototransformation rate $k = 0.015 \text{ h}^{-1}$ with $t_{1/2} = 46$ h in the summer (mean temp 24°C) and $k = 0.0040 \text{ h}^{-1}$ with $t_{1/2} = 173$ h in the winter (mean temp 10°C) in distilled water; $k = 0.018 \text{ h}^{-1}$ with $t_{1/2} = 39$ h in the summer and $k = 0.0074 \text{ h}^{-1}$ with $t_{1/2} = 94$ h in the winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);

photomineralization rate $k = 0.04 \text{ h}^{-1}$ with $t_{1/2} = 16$ d in the summer and $k = 0.0041 \text{ h}^{-1}$ with $t_{1/2} = 169$ d in the winter in distilled water; $k = 0.095 \text{ h}^{-1}$ with $t_{1/2} = 7$ d in the summer and $k = 0.010 \text{ h}^{-1}$ with $t_{1/2} = 73$ d in winter in estuarine water when exposed to full sunlight and microbes (Hwang et al. 1986);

atmospheric $t_{1/2} = 46$ to 173 h, based on reported half-life for photolysis under sunlight for phenol in distilled water in the summer and winter; aquatic photolysis $t_{1/2} = 46$ to 173 h, based on reported half-life for photolysis under sunlight for phenol in distilled water in the summer and winter (Howard et al. 1991)

Apparent first-order rate constant phototransformation at $\lambda > 285 \text{ nm}$, $k = (3.10 \pm 0.10) \times 10^{-2} \text{ h}^{-1}$ in purified water (Zamy et al. 2004)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k = 1 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 0.8$ d (Howard 1972; Hendry et al. 1974; quoted, Mill 1982)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen at 25°C with $t_{1/2} > 100$ yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{\text{NO}_3} = (2.0 \pm 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(300 \pm 1) \text{ K}$ (Carter et al. 1981)

$k = 6.5 \times 10^3 \text{ s}^{-1}$, dye-sensitized photooxidation first-order rate constant, second order $k = (1.3 \pm 0.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM PrOH as scavenger at pH 1.7–2.0 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983a)

$k_{\text{NO}_3} = (2.10 \pm 0.50) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1984)

$k_{\text{NO}_3} = (3.64 \pm 0.14) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K with reference to reaction for NO_3 radical with 2-methyl-2-butene (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{OH}}(\text{exptl}) = 28.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 45.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985)

$k_{\text{OH}}(\text{calc}) = 36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{obs}) = 28.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k = (2 \text{ to } 3) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, $1.9 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9, $4.6 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9.5, $9.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 10 and $1.8 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 11.5 for the reaction with singlet oxygen at $(19 \pm 2)^\circ\text{C}$ in water (Scully & Hoigné 1987)

$k_{\text{NO}_3} = 3.63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güsten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 26.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{NO}_3} = (2.59 \pm 0.52) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ with reference to reaction for NO_3 radicals with *cis*-2-butene (Atkinson 1991)

$k = (2.6 \pm 4) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $(27 \pm 1)^\circ\text{C}$ (Tratnyek & Hoigné 1991)

$k_{\text{OH}} = 10.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{NO}_3} = 11.44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Müller & Klein 1991)

$k_{\text{NO}_3} = (3.92 \pm 0.25) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ with reference to reaction for NO_3 radical with 2-methyl-2-butene; $k_{\text{OH}} = 26.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1992)

$k_{\text{OH}}(\text{calc}) = 12 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

$k_{\text{OH}} = 2.6 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{aq.}) = 6.7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.45 \text{ d}$ under clear sky; $\tau = 0.38 \text{ d}$ under cloudy conditions at 298 K , reduced to 0.26 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis: no hydrolyzable function group (Howard et al. 1991).

Biodegradation: $t_{1/2} = 1\text{--}2 \text{ d}$ for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964)

decomposition by soil microflora within 1 d (Alexander & Lustigman 1966; quoted, Verschueren 1983)

complete disappearance in soil suspensions in 2 d (Woodcock 1971; quoted, Verschueren 1983)

$k_{\text{B}} = 80.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

$k_{\text{B}} = (0.094 \pm 0.003) \text{ h}^{-1}$ at feed concentration of 180 mg/L at 20°C and $k = (0.095 \pm 0.007) \text{ h}^{-1}$ at feed concentration of 360 mg/L at 20°C in a continuous stirred reactor (Beltrame et al. 1984)

$k_{\text{B}} = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 20 \text{ d}$ in ground water; $k_{\text{B}} = 0.065 \text{ d}^{-1}$ with $t_{1/2} = 11 \text{ d}$ in Lester River water;

$k_{\text{B}} = 0.247 \text{ d}^{-1}$ with $t_{1/2} = 3 \text{ d}$ in Superior harbor waters (Vaishnav & Babeu 1987)

$k_{\text{B}} = 0.03 \text{ h}^{-1}$ and $t_{1/2} = 28 \text{ h}$ for estuarine water in summer (mean temp 24°C) and $k_{\text{B}} = 0.011 \text{ h}^{-1}$ with $t_{1/2} = 62 \text{ h}$ in winter (mean temp. 10°C); $k_{\text{B}} = 0.4 \text{ h}^{-1}$ with $t_{1/2} = 2 \text{ d}$ in summer and $k_{\text{B}} = 0.0051 \text{ h}^{-1}$ with $t_{1/2} = 146 \text{ d}$ in winter in darkness with microbes (Hwang et al. 1986)

$k_{\text{B}} = 0.041\text{--}0.028 \text{ h}^{-1}$ in $10\text{--}100 \text{ mg/L}$ sludge (Urano & Kato 1986)

complete degradation within 1 d in water from 3 lakes, and degradation is somewhat slower in salt water with $t_{1/2} = 9 \text{ d}$ in estuary river (Howard 1989)

$k_{\text{B}}(\text{exptl., average}) = 0.0498 \text{ h}^{-1}$; $k_{\text{B}}(\text{calc}) = 0.0545 \text{ h}^{-1}$ (nonlinear) and $k_{\text{B}}(\text{calc}) = 0.0503 \text{ h}^{-1}$ (linear) (group contribution method, Tabak & Govind 1993)

$t_{1/2}(\text{aerobic}) = 0.25 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8.0 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: microbial transformation $k = (7.1 \pm 1.3) \times 10^{-12} \text{ L.organism}^{-1} \text{ h}^{-1}$ (Paris et al. 1982);

estimated bacterial transformation $k = 3 \times 10^{-6} \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);

microbial transformation rate constants in pond and river samples $k = (2.0 \pm 1.5) \times 10^{-10}$ to $(4.8 \pm 3.1) \times 10^{-10} \text{ L organism}^{-1} \text{ h}^{-1}$ at five different sites (Paris et al. 1983; quoted, Steen 1991);

degradation rate constants $k = 1.08 \times 10^{-16} \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies and $k = 0.90 \times 10^{-12}$ to $3.00 \times 10^{-12} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 3.15 \text{ h}^{-1}$; $k_2 = 0.02 \text{ h}^{-1}$ (goldfish, Nagel & Urich 1980)

Half-Lives in the Environment:

Air: $t_{1/2} = 0.61 \text{ d}$ by reaction with OH radicals in air (Howard 1989);

$t_{1/2} = 2.28$ to 22.8 h , based on reaction with OH radical (Howard et al. 1991)

degradation $k = 0.0462 \text{ d}^{-1}$ corresponding to $t_{1/2} = 360 \text{ h}$ in air (Guinee & Heijungs 1993);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994);

calculated lifetimes of 5.3 h and 9.0 min for reactions with OH, NO_3 radical, respectively (Atkinson 2000).

atmospheric lifetime $\tau = 0.45 \text{ d}$ under clear sky and $\tau = 0.38 \text{ d}$ under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K , reduced to $\tau = 0.26 \text{ d}$ due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: rate constant $k = (1.3 \pm 0.2) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 2.0–6.0 (Hoigné & Bader 1983);

$t_{1/2} = 46 \text{ h}$ in summer, $t_{1/2} = 173 \text{ h}$ in winter in distilled water and $t_{1/2} = 39 \text{ h}$ in summer, $t_{1/2} = 94 \text{ h}$ in winter in estuarine water, based on phototransformation rate when exposed to full sunlight and microbes (Hwang et al. 1986)

$t_{1/2} = 43 \text{ h}$ in summer, $t_{1/2} = 118 \text{ h}$ in winter in poisoned estuarine water, based on photo-transformation rate and $t_{1/2} = 384 \text{ h}$ or 16 d in summer, $t_{1/2} = 2640 \text{ h}$ or 110 d in winter in poisoned estuarine water, based on photomineralization rate (Hwang et al. 1986);

$t_{1/2}$ = 384 h or 16 d in summer, $t_{1/2}$ = 4056 h or 169 d in winter in distilled water; and $t_{1/2}$ = 168 h or 7 d in summer, $t_{1/2}$ = 1752 h or 73 d in winter in estuarine water, based on photo-mineralization rate when exposed to full sunlight and microbes (Hwang et al. 1986);

$t_{1/2}$ = 2000 h in water at pH 8 and $19 \pm 2^\circ\text{C}$ for the reaction with singlet oxygen (Scully & Hoigné 1987); biodegradation $t_{1/2}$ = 11 d in river waters and $t_{1/2}$ = 3 d in Superior harbor waters (Vaishnav & Babeu 1987); complete degradation within 1 d in water from 3 lakes, and degradation is somewhat slower in salt water with $t_{1/2}$ = 9 d in estuary river (Howard 1989);

$t_{1/2}$ = 77 to 3840 h in water, based on reported reaction rate constant for RO_2 radical with the phenols class, $t_{1/2}$ = 5.3 to 56.5 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991); degradation rate constant $k = 0.0217 \text{ d}^{-1}$ corresponding to a $t_{1/2}$ = 766 h in water (quoted from Howard 1989, Guinee & Heijungs 1993)

$t_{1/2}(\text{aerobic}) = 0.25 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 8 \text{ d}$ in natural waters (Capel & Larson 1995)

Groundwater: biodegradation $t_{1/2}$ = 20 d (Vashnav & Babeu 1987);

$t_{1/2}$ = 12 to 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 2 d in Dunkirk silt loam, 1 d in Mardin silt loam (Alexander & Aleem 1961)

degradation in soil completed in 2–5 d even in subsurface soils and $t_{1/2}$ = 2.70 and 3.51 h of low concentration of phenol in 2 silt loam soils (Howard 1989);

$t_{1/2}$ = 24 to 240 h, based on aerobic soil die-away data (Howard et al. 1991);

$t_{1/2}$ = 4.1 d in a slightly basic sandy loam soil containing 3.25% organic matter and $t_{1/2}$ = 23 d in acidic clay soil with < 1.0% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992)

degradation rate constant $k = 0.227 \text{ d}^{-1}$ corresponding to a $t_{1/2}$ = 73.3 h in soil (quoted from Howard 1989, Guinee & Heijungs 1993).

Biota: elimination from goldfish within 4 h (Nagel & Ulrich 1980);

depuration $t_{1/2}(\text{obs}) = 336 \text{ h}$, $t_{1/2}(\text{calc}) = 385 \text{ h}$ for exposure level of $0.0025 \mu\text{g mL}^{-1}$ and $t_{1/2}(\text{obs.}) = 438 \text{ h}$, $t_{1/2}(\text{calc}) = 497 \text{ h}$ for exposure level of $0.0375 \mu\text{g mL}^{-1}$ (Call et al. 1980);

depuration $t_{1/2}(\text{calc}) = 8$ to 44 min in algae (Hardy et al. 1985);

half-lives in fish $t_{1/2} < 1 \text{ d}$ for goldfish, $t_{1/2} = 14$ –18 d for minnow (Niimi 1987)

TABLE 14.1.1.1.1

Reported aqueous solubilities of phenol at various temperatures

1.

Hill & Malisoff 1926		Morrison 1944		Erichsen & Dobbert 1955		Achard et al. 1996	
volumetric method		thermostatic and synthetic		shake flask-optical method		shake flask-conductivity	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
20.0	83600	22.7	89300	0	73000.	15.1	76044
25.0	86600	26.9	93159	10	75000	25.0	84045
30.0	92200	32.3	98617	20	79000	35.0	93098
35.0	99100	36.0	104169	30	86000		
57.30	148700	43.7	108968	40	97000		
62.74	193500	47.7	128823	50	115000		
65.79	277700	50.5	138892	60	153000		
66.01	291300	53.5	149807	62	166000		
65.79	202100	55.8	162323	64	183000		
65.84	313500	57.8	174650	66	215000		
65.86	322300	60.9	203538	67	252000		
65.84	327900			68	316000		
				68.3	365000		

(Continued)

TABLE 14.1.1.1.1 (Continued)

2.

Jaoui et al. 1999		Jaoui et al. 2002	
static visual method		static visual method*	
T/K	S/g·m ⁻³	T/K	S/g·m ⁻³
298.5	94100	292.5	81011
307.5	99328	296.1	82959
313.4	104556	296.3	83119
313.7	143764	300.2	86290
319.8	118149	302.7	88341
324.8	134877	305.8	90901
331.5	151606	308.4	93065
336.7	182970	313.3	97186
		315.4	100169
		322.4	114416
		326.8	124024
		331.3	134394
		333.6	139814

some data from Achard et al.
1996, Jaoui et al. 1999

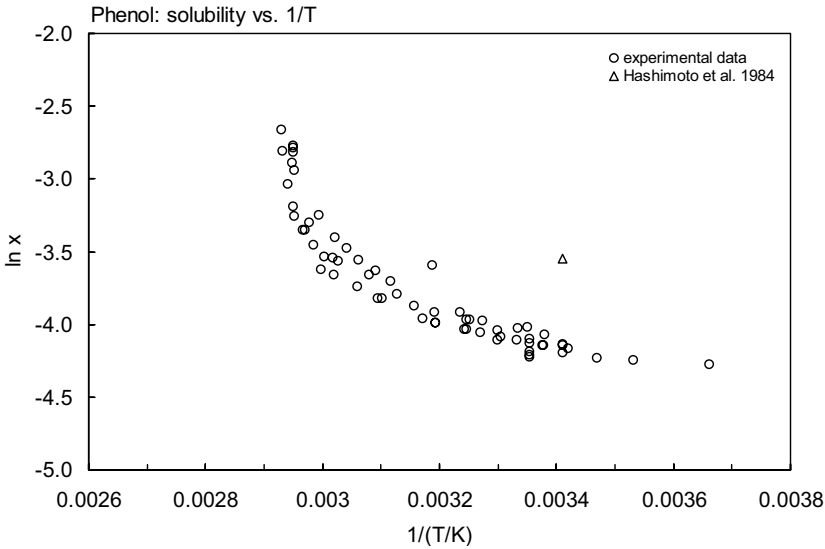


FIGURE 14.1.1.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for phenol.

TABLE 14.1.1.1.2

Reported vapor pressures of phenol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Kahlbaum 1898*		Stull 1947		Goldblum et al. 1947		Dreisbach & Shrader 1949	
static-manometer		summary of literature data		mercury manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
44.8	133.3	40.1	133.3	141.1	28531	107.15	7605
51.5	266.6	62.5	666.6	152.6	42263	113.81	10114
55.8	400.0	73.8	1333	164.4	61061	125.95	16500
59.3	533.3	86.0	2666	168.3	68661	152.37	42066
62.5	666.6	100.1	5333	173.5	80127	167.63	67661
73.5	1333.2	108.4	7999	181.0	98659	181.75	101325
85.8	2666.4	121.4	13332	140.2	27598		
93.8	3999.7	139.0	26664	145.1	32797	bp/°C	181.75
99.8	5533	160.0	53329	171.4	75194		
104.4	6661	181.9	101325	176.6	87060		
113.7	9992			181.1	98525		
120.2	13332	mp/°C	40.6				
139.0	26664			eq. 1	P/mmHg		
151.0	39997			A	8.395		
160.0	53329			B	2510		
167.0	66661						
173.0	79993						
179.0	93326						
181.4	101325						

*complete list see [ref.](#)

2.

Vonterres et al. 1955		Biddiscombe & Martin 1958				Tabai et al. 1997	
ebulliometry		gas saturation/diaphragm manometer				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		solid		liquid			
70.50	1333	0	3.746	121.25	13583	40.09	173
90.20	3333	5.1	6.159	131.183	20005	50.0	345
104.2	6666	9.25	9.413	138.014	25635	60.0	655
113.0	9999	9.85	10.40	140.704	28226	70.03	1187
121.5	13332	10.4	10.47	147.204	35310	79.97	2048
132.5	19998	14.5	16.0	155.343	46139	89.99	3415
140.1	26664	18.25	22.93	156.196	47902		
147.0	33330	18.25	23.20	156.528	53130		
152.0	39997	19.6	26.66	159.799	54843		
153.0	43330	22.0	35.60	160.124	58843		
156.0	46663	24.85	44.26	163.795	60104		
160.0	53329	28.15	63.73	168.945	70154		

(Continued)

TABLE 14.1.1.1.2 (Continued)

Vonterres et al. 1955		Biddiscombe & Martin 1958				Tabai et al. 1997	
ebulliometry		gas saturation/diaphragm manometer				ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
164.0	59995	30.5	74.39	169.991	72357		
167.0	73327	32.95	92.93	171.025	74590		
170.5	73327	35.0	108.5	172.635	78154		
173.0	79993	37.45	138.7	173.066	79148		
176.0	86659			175.767	85526		
179.0	93325	bp/°C	181.839	178.196	91590		
181.7	101325			179.878	94918		
		Antoine eq. for temp range:		180.863	98625		
		0–40°C		181.551	100497		
		eq. 1	P/mmHg	182.053	101904		
		A	11.5638				
		B	3586.36	Antoine eq. for temp range:			
		C	273	110–200°C			
				eq. 2	P/mmHg		
		ΔH_v /(kJ mol ⁻¹)		A	7.13457		
		at bp	47.304	B	1516.072		
		at 25°C	68.66	C	174.569		

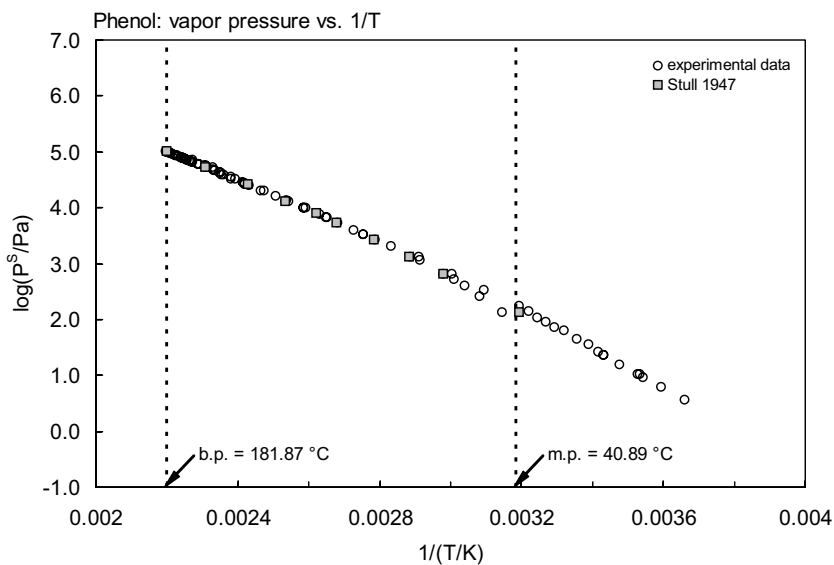


FIGURE 14.1.1.1.2 Logarithm of vapor pressure versus reciprocal temperature for phenol.

TABLE 14.1.1.1.3

Reported Henry's law constants of phenol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)		
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)		
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)					
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)		
$\ln k_H = A - B/(T/K) - C \cdot \ln (T/K)$		(5)					
Abd-El-Bary et al. 1986		Dohnal & Fenclová 1995		Tabai et al. 1997		Feigenbrugel et al. 2004	
gas stripping-GC/FID		vapor-liquid equilibrium		derived from measured P		gas stripping-GC/MS	
t/°C	H/(Pa m³/mol)	t/°C	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)	T/K	H/(Pa m³/mol)
−2.0	0.0072	4.0	0.0127*	313.24	0.0342	278.15	0.0222
4.0	0.0127	18.3	0.0373*	323.15	0.090	278.15	0.0299
18.3	0.0373	27.0	0.0721*	333.15	0.202	278.20	0.0280
27.0	0.0718	80.3	1.552*	343.18	0.355	278.25	0.0337
44.4	0.193*	100.0	3.537*	353.12	0.506	283.05	0.0340
56.3	0.437*	75.9	1.245	363.14	0.999	283.15	0.0456
75.0	1.233*	88.7	2.193			283.15	0.0328
90.0	2.376*	98.6	3.322	eq. 5	k _H /kPa	283.25	0.0428
		25.0	0.0607#	A	670.117	283.25	0.0404
*data from literature		25.0	0.0605\$	B	29374.5	288.15	0.0590
			#calculated from eq. 1	C	94.6679	288.15	0.0928
			\$calculated from eq. 3	temp range 313–363 K		288.25	0.0560
			*data from literature			293.15	0.1166
eq. 3	k _H /kPa					293.15	0.169
A	21.7128	eq. 1	K _{AW}	Harrison et al. 2002		293.15	0.1093
B	6120.0	A	8.701	gas stripping-UV		293.15	0.1065
eq. derived included lit. data		B	5760	T/K	H/(Pa m³/mol)	293.25	0.0960
		enthalpy of hydration:				293.25	0.1071
		$\Delta H_K/(\text{kJ mol}^{-1}) = 47.9 \pm 0.5$		284	0.0122	298.15	0.0904
		OR		284.5	0.0110	298.15	0.2022
		eq. 3	k _H /kPa	289.5	0.0199	298.15	0.1375
		A	21.443	293.5	0.0262		
		B	6032	298	0.0320		
		$\Delta H_K/(\text{kJ mol}^{-1}) = 50.2 \pm 0.4$		302	0.0379		
				eq. 4	H/(M atm ^{−1})		
				A	−11.6		
				B	−5850		

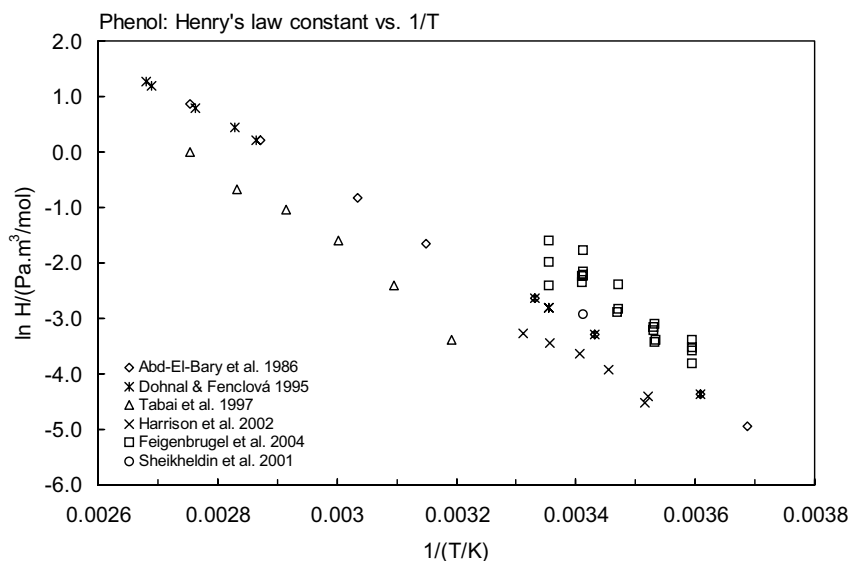


FIGURE 14.1.1.1.3 Logarithm of Henry's law constant versus reciprocal temperature for phenol.

TABLE 14.1.1.1.4

Reported octanol-water partition coefficients of phenol at various temperatures

Korenman & Udalova 1974

shake flask-concn ratio	
t/°C	log K _{OW}
10	1.531
20	1.510
30	1.461
40	1.433
50	1.396
60	1.369
log K _{OW} = A – B/(T/K)	
A	0.4479
B	–305.877

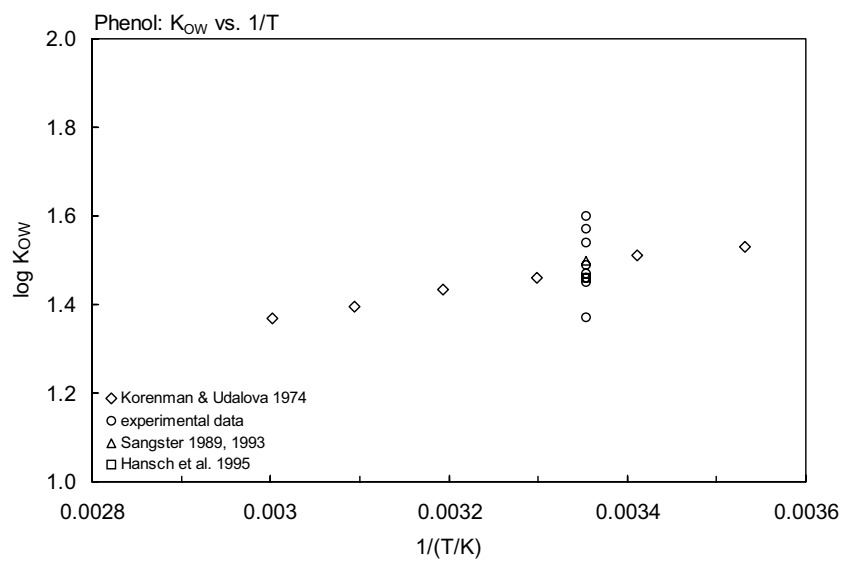
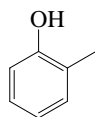


FIGURE 14.1.1.1.4 Logarithm of K_{OW} versus reciprocal temperature for phenol.

14.1.1.2 *o*-Cresol

Common Name: *o*-Cresol

Synonym: 2-hydroxytoluene, 2-methylphenol, *o*-cresylic acid, *o*-hydroxytoluene, 2-cresol, 1,2-cresol

Chemical Name: 2-methylphenol

CAS Registry No: 95-48-7

Molecular Formula: C_7H_8O , $C_6H_4(CH_3)OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

31.03 (Lide 2003)

Boiling Point ($^{\circ}C$):

191.04 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0273 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

10.28 (Pearce & Simkins 1968)

10.20 (Hoigné & Bader 1983; Weast 1982–83)

10.26 (Dean 1985)

Molar Volume (cm^3/mol):

104.4 ($30^{\circ}C$, Stephenson & Malanowski 1987)

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

46.94 (Biddiscombe & Martin 1958)

45.91 (at normal boiling point, Andon et al. 1960)

42.7 (Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

76.02 (at $25^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.8 (Tsonopoulos & Prausnitz 1971; Riddick et al. 1986)

Entropy of Fusion ΔS_{fus} ($J/mol K$):

52.01 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F : 0.873 (mp at $31.03^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

30100* ($35.3^{\circ}C$, shake flask, measured range 35.3 – $162.8^{\circ}C$, critical solution temp $162.8^{\circ}C$, Sidgwick et al. 1915)

24970 (shake flask-residue volume method, Booth & Everson 1948)

25950 (shake flask-UV at pH 5.1, Blackman et al. 1955)

25000* ($20^{\circ}C$, synthetic method/shake flask-optical, measured range 0 – $166.5^{\circ}C$, Ericksen & Dobbert 1955)

25000 (shake flask-UV spectrophotometry, Roberts et al. 1977)

2725 (generator column-HPLC, Wasik et al. 1981)

31000, 56000 ($40^{\circ}C$, $100^{\circ}C$, Verschueren 1983)

42608, 48061, 52241 (75.9 , 88.7 , $98.5^{\circ}C$, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

26820* (calculated-activity coeff. γ^{∞} data, measured range 25 – $35^{\circ}C$, Dohnal & Fenclová 1995)

26800 (shake flask-HPLC/UV at pH 3.6, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

23065* ($142.3^{\circ}C$, mercury manometer, measured range 142.3 – $190.8^{\circ}C$, Goldblum et al. 1947)

- $\log (P/\text{mmHg}) = -2520/(T/K) + 8.308$; temp range 142.3–177.1°C (Hg manometer, Goldblum et al. 1947)
 58.16* (extrapolated-regression of tabulated data, temp range 38–190.5°C, Stull 1947)
 7605* (113.11°C, ebulliometry, measured range 113.11–190.95°C, Dreisbach & Shrader 1949)
 56.72 (calculated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 7.49476 - 1777.8/(203.0 + t/^{\circ}\text{C})$; temp range 97–250°C (Antoine eq. for liquid state, Dreisbach 1955)
 38.60 (gas saturation and diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
 37.32* (25.25°C, gas saturation -diaphragm manometer, temp range 0–28°C, Biddiscombe & Martin 1958)
 $\log (P/\text{mmHg}) = 12.7778 - 3970.17/(t/^{\circ}\text{C} + 273)$; temp range 0–30°C (Antoine eq. gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P/\text{mmHg}) = 7.07055 - 1542.299/(t/^{\circ}\text{C} + 177.110)$; temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P/\text{mmHg}) = [-0.2185 \times 12487.3/(T/K)] + 8.79055$; temp range 38.2–190.8°C (Antoine eq., Weast 1972–73)
 30.7 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 6.91172 - 1435.503/(165.158 + t/^{\circ}\text{C})$; temp range 120–191°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
 32.0 (Verschuere 1977, 1983)
 38.32 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 463.986/(T/K)] \times 10^{\{1.01555 - 9.95980 \times 10^{-4} \cdot (T/K) + 7.92834 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 313.20–697.65 K (Cox eq., Chao et al. 1983)
 30.3, 22.5 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.02377 - 1427.165/(164.218 + t/^{\circ}\text{C})$; temp range 120–191°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 5.82809 - 1299.971/(148.886 + t/^{\circ}\text{C})$; temp range 142.3–189.8°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 30.74 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 6.9117 - 1435.5/(165.16 + t/^{\circ}\text{C})$; temp range 120–191°C (Antoine eq., Dean 1985, 1992)
 37.70 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.68858 - 3909.409/(T/K)$; temp range 273–303 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19545 - 1542.299/(-96.04 + T/K)$; temp range 383–473 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.47616 - 1714.489/(-79.841 + T/K)$; temp range 304–409 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19561 - 1543.097/(-95.902 + T/K)$; temp range 399–470 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24893 - 1584.403/(-90.794 + T/K)$; temp range 463–526 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.82237 - 2134.352/(-19.536 + T/K)$; temp range 517–630 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)
 40.0 (Riddick et al. 1986)
 39.4 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 99.85294 - 6347.665/(T/K) - 32.60231 \cdot \log (T/K) + 1.24267 \times 10^{-2} \cdot (T/K)$; temp interval of investigation: 412–467 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 89.4591 - 6.0489 \times 10^3/(T/K) - 29.481 \cdot \log (T/K) + 1.0936 \times 10^{-4} \cdot (T/K) + 1.9933 \times 10^{-12} \cdot (T/K)^2$; temp range 304–698 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.124, 0.07, 1.082 (exptl., calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 0.284, 0.162 (8, 25°C, calculated, Leuenberger et al. 1985)
 0.0852 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
 0.176* (°C, calculated-activity coeff. γ^{∞} data, measured range 25–35°C, Dohnal & Fenclová 1995)

3.352, 5.386, 8.652 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.178 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 9.091 - 5556/(T/K)$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 0.159 (gas stripping-GC, Altschuh et al. 1999)
 0.102 (calculated-group contribution, Lee et al. 2000)
 0.217 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
 0.0965* (gas stripping-UV, measured range 281–302 K, Harrison et al. 2002)
 $\ln [H/(M \text{ atm}^{-1})] = 6680/(T/K) - 15.4$; temp range 281–302 K, Harrison et al. 2002)
 0.146, 0.239* (20, 25°C, dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.04 (shake flask-UV, Korenman & Pereshein 1970)
 1.95 (from Hansch & Dunn III unpublished result, Leo et al. 1971; Hansch & Leo 1985)
 1.95 (LC- k' correlation, Carlson et al. 1975)
 2.045 (shake flask, Korenman et al. 1980)
 2.17 (HPLC- k' correlation, Butte et al. 1981; Butte et al. 1987)
 1.96 (generator column-HPLC, Wasik et al. 1981)
 1.99 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.98 (recommended, Sangster 1989)
 1.97, 1.98 (COMPUTOX data bank, Kaiser 1993)
 1.95 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.26 (calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
 1.03 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

1.34 (Brookstone clay loam soil at pH 5.7, Boyd 1982; quoted, Howard 1989)
 1.26 (calculated-S, Boyd 1982; quoted, Howard 1989)
 1.76 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 3.41 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (relative rate method with reference 2-methyl-2-butene Perry et al. 1977; Atkinson et al. 1979)

$k_{NO_3} = (12 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (relative rate method with reference to with 2-methyl-2-butene Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for oxidation with singlet oxygen at 25°C in the aquatic system with half-life > 100 yr (Foote 1976; Mill 1979; quoted, Mill 1982)

$k_{OH} = 20 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C with $t_{1/2} = 0.3 \text{ d}$ (Hendry & Kenley 1979; quoted, Mill 1982)

$k_{NO_3} = (13.9 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $300 \pm 1 \text{ K}$ (relative rate method with reference to the reaction of NO_3 radical with 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)

photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reaction rate constants for OH and RO_2 radicals with the phenol class (Güsten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991)

$k_{O_3} = (2.55 \pm 0.39) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$; calculated tropospheric lifetimes of 45 d and 0.3 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

$k_{OH} = 2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ with half-life of 0.3 d in the atmosphere (Mill 1982)

$k_{OH} = 2.0 \times 10^{13} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 300 K (Lyman et al. 1982)

$k = (1.2 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.5–2.0 (Hoigné & Bader 1983b)

$k_{\text{OH}} = 4.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{\text{NO}_3} = 1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = (1.20 \pm 0.34) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1984)

$k_{\text{NO}_3} = (15.6 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of NO_3 radical with *m*-cresol at $(298 \pm 1) \text{ K}$ (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{NO}_3} = 22 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with $2.4 \times 10^8 \text{ NO}_3 \text{ radical/cm}^3$ at room temp. and a loss rate of 450 d^{-1} with $t_{1/2} = 1.6\text{--}16 \text{ h}$ (Atkinson et al. 1984, 1985; quoted, Atkinson 1985)

$k_{\text{OH}} = 40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with $5 \times 10^5 \text{ hydroxyl radical/cm}^3$ at room temp. and a loss rate of 1.7 d^{-1} (Atkinson 1985; quoted, Howard et al. 1991)

$k_{\text{OH}}(\text{exptl}) = 37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{calc}) = 44.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}}(\text{exptl}) = 40 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{calc}) = 44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 4.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k_{\text{NO}_3} = (13.7 \pm 0.9) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(296 \pm 2) \text{ K}$, and $k_{\text{OH}} = 42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for at room temp. (Atkinson et al. 1992)

$k_{\text{OH}}(\text{calc}) = 30.36 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}} = 4.9 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{aq.}) = 1.1 \times 10^{-10} \text{ M}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.24 \text{ d}$ under clear sky; $\tau = 0.22 \text{ d}$ under cloudy conditions at 298 K, reduced to 0.17 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis:

Biodegradation: 1 to 2 d for bacteria to utilize 95% of 300 ppm in the parent substrate (Tabak et al. 1964)

$t_{1/2} = 2 \text{ d}$ at 20°C and 7 d at 4°C in river water (Ludzack & Ettinger 1960; quoted, Howard 1989)

completely degraded by a soil microflora within one day (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation $k = 54.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on unacclimated aerobic screening test data (Takemoto et al. 1981; Urushigawa et al. 1983; quoted, selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$k(\text{exptl.}) = 0.0679 \text{ h}^{-1}$ compared to group contribution method predicted $k(\text{calc}) = 0.0728 \text{ h}^{-1}$ (nonlinear) and $k = 0.0567 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 15 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: microbial transformation $k = (2.7 \pm 1.3) \times 10^{-10} \text{ L-organism}^{-1} \text{ h}^{-1}$ (Paris et al. 1983; quoted, Steen 1991).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1.6\text{--}16 \text{ h}$ in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991);

loss rate $k = 10.8 \times 10^{-4} \text{ min}^{-1}$ in outdoor Teflon chambers in the dark (Grosjean 1985);

photodegradation $t_{1/2} \sim 9.6 \text{ h}$ in air, based on measured rate constant for the reaction with photochemically generated hydroxyl radicals (quoted, Howard 1989);

atmospheric transformation lifetime $\tau < 1 \text{ d}$ (estimated, Kelly 1994);

calculated lifetimes of 2.2 h, 2 min and 65 d for reactions with OH radical, NO_3 radical and O_3 , respectively (Atkinson 2000).

calculated atmospheric lifetime $\tau = 0.24 \text{ d}$ under clear sky and $\tau = 0.22 \text{ d}$ under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to $\tau = 0.19 \text{ d}$ due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reaction rate constants for OH and RO_2 radicals with the phenol class (Güesten et al. 1981; Mill & Mabey 1985; quoted, Howard et al. 1991)

rate constant $k = (1.2 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983)

$t_{1/2}(\text{aerobic}) = 2 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 15 \text{ d}$ in natural waters (Capel & Larson 1995)

Ground water: estimated $t_{1/2} \sim 0.01 \text{ yr}$ for cresols at Noordwijk (Zoeteman et al. 1981).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2} = 5.1$ d in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 1.6$ d in slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.1.2.1

Reported aqueous solubilities of *o*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Dohnal & Fenclová 1995	
shake flask-synthetic method		shake flask-optical method		vapor-liquid equil.-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
35.3	30100	0	22000	25	26820
50.2	32200	20	25000	30	28470
61.7	34700	40	28000	35	30810
70.6	37500	60	32000	75.9	42608
77.7	41000	80	38000	88.7	48061
84.6	45100	100	48000	98.5	52241
130.6	65200	120	67000	100	53640
148.7	104600	130	82000		
158.7	193600	140	102000		
161.7	300600	150	136000		
162.8	408900	160	202000		
160.0	501400	162	228000		
157.7	598000	164	275000		
145.7	693000	166	352000		
129.6	761400	166.5	400000		
87.5	823700				
56.6	845800				
33.6	866000				
25.6	861400				
8.3	875200				
9.1	886800				
10.2	898900				
11.1	908500				
12.9	926200				
15.3	940800				
22.3	974600				
26.9	990100				
29.9	1000000				
critical solution temp 162.8°C					
triple point 8°C					

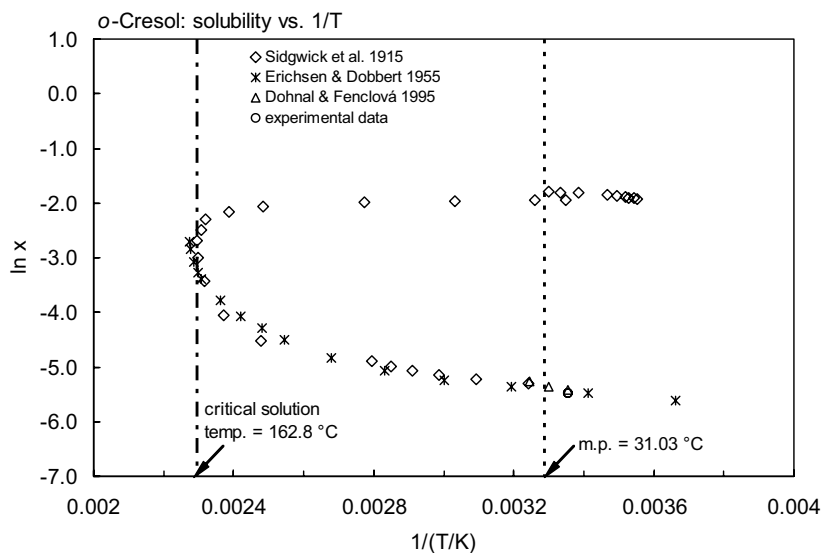


FIGURE 14.1.1.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *o*-cresol.

TABLE 14.1.1.2.2

Reported vapor pressures of *o*-cresol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$	(3)		
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$	(4)		

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
							solid		liquid
38.2	133.3	142.3	23065	113.11	7605	0	2.680	138.575	20410
64.0	666.6	153.3	33731	120.22	10114	2.90	2.093	146.128	26548
76.7	1333	164.5	47729	132.63	16500	5.0	4.213	152.680	33025
90.5	2666	171.2	58529	160.17	42066	5.60	4.680	158.592	39922
105.8	5333	183.5	81993	176.14	67661	9.80	6.933	163.551	46571
115.5	7999	189.8	97859	190.95	101325	10.05	7.773	168.080	53394
127.4	13332	143.7	24265			14.85	13.20	172.002	59935
146.7	26664	166.8	51329			14.90	12.60	175.642	66563
168.4	53329	172.0	61328	bp/°C	190.95	17.40	18.27	179.039	73277
190.8	101325	179.4	73861			19.50	22.0	182.183	79956
		177.1	69194			20.0	22.40	185.185	86782
mp/°C	30.8					20.35	22.66	187.735	92934
						24.35	34.66	188.487	94810
						25.25	37.33	189.013	96149
		eq. 1	P/mmHg			26.65	45.20	189.455	97276
		A	8.308			27.25	48.40	189.973	98613
		B	2520			28.35	66.66	190.371	99650
								190.486	99953
						mp/°C	30.99	190.545	100125

(Continued)

TABLE 14.1.1.2.2 (Continued)

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						bp/°C	191.003	191.046	101452
								191.135	101668
						for temp range:		191.511	102686
						0–30°C			
						eq. 2	P/mmHg		
						A	11.5638	for temp range:	
						B	3586.36	110–200°C	
						C	273	eq. 2	P/mmHg
								A	7.13457
								B	1516.072
						ΔH _v /(kJ mol ⁻¹)		C	174.569
						at bp	46.94		
						at 25°C	76.02		

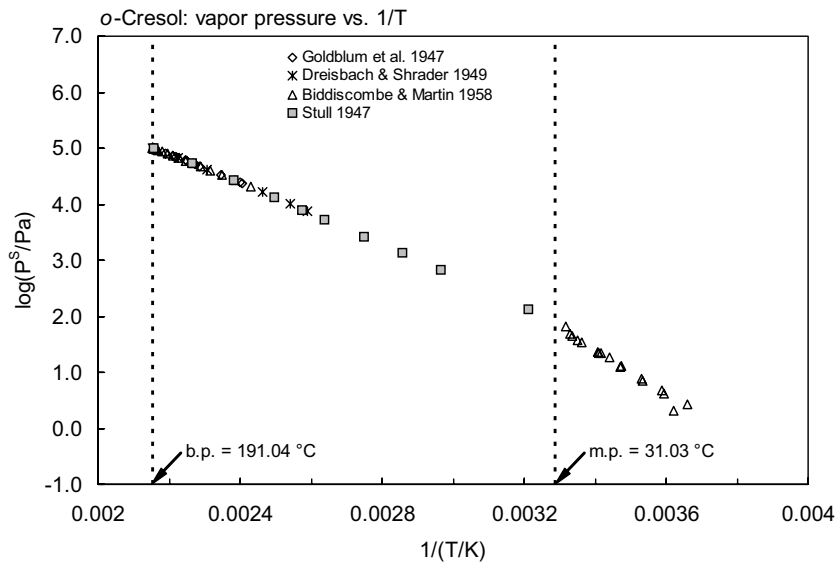
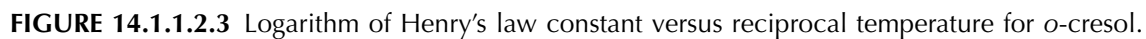


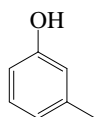
FIGURE 14.1.1.2.2 Logarithm of vapor pressure versus reciprocal temperature for *o*-cresol.

TABLE 14.1.1.2.3

Reported Henry's law constants of *o*-cresol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
Dohnal & Fenclová 1995		Harrison et al. 2002		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-UV		gas stripping-GC/MS	
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)
25	0.176*	281	0.0224	278.25	0.0348
30	0.245*	284.5	0.0313	278.25	0.0355
35	0.341*	289.5	0.0596	278.35	0.0286
75.9	3.352	293.5	0.0650	283.15	0.0707
88.7	5.386	298	0.0965	283.15	0.0556
98.5	8.652	302	0.1165	283.25	0.0565
100	9.028			288.10	0.0842
25.0	0.1777#	eq. 4	H/(M atm ⁻¹)	288.15	0.1137
25.0	0.1764\$	A	-15.4	288.20	0.0855
		B	-6680	293.10	0.1603
#calculated from eq. 1				293.15	0.1626
\$calculated from eq. 3				293.15	0.1554
*data from literature				293.15	0.1371
				293.15	0.1883
eq. 1	K _{AW}			293.25	0.1537
A	9.091			298.15	0.2356
B	5556			298.15	0.2362
enthalpy of hydration:				293	0.1464
ΔH _K /(kJ mol ⁻¹) = 46.2 ± 0.4				298	0.2390
OR					
eq. 3	k _H /kPa				
A	21.832				
B	5827				
ΔH _K /(kJ mol ⁻¹) = 48.5 ± 0.4					



14.1.1.3 *m*-Cresol

Common Name: *m*-Cresol

Synonym: *m*-cresylic acid, 1-hydroxy-3-methylbenzene, 3-hydroxytoluene, *m*-hydroxytoluene, 3-methylphenol, *m*-methylphenol, 3-cresol

Chemical Name: *m*-cresol, 3-methylphenol

CAS Registry No: 108-39-4

Molecular Formula: C_7H_8O , $C_6H_4(CH_3)OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

12.24 (Lide 2003)

Boiling Point ($^{\circ}C$):

202.27 (Lide 2003)

Density (g/cm^3):

1.0336 (Weast 1982–83)

1.0302 (25 $^{\circ}C$, Riddick et al. 1986)

Acid Dissociation Constant, pK_a :

10.09 (Pearce & Simkins 1968; Riddick et al. 1986; Howard 1989)

10.0 (Hoigné & Bader 1983; Dean 1985)

10.01 (Weast 1982–83)

Molar Volume (cm^3/mol):

105.6 (calculated-density, Rohrschneider 1973)

125.6 (calculated-Le Bas-method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.38 (at normal bp, Biddiscombe & Martin 1958)

47.40 (at normal boiling point, Andon et al. 1960)

61.714 (at 25 $^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

6.53 (Tsonopoulos & Prausnitz 1971)

10.70 (Riddick et al. 1986; Dean 1992)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

37.53 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 1.0

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

23600* (24.7 $^{\circ}C$, shake flask, measured range –2 to 87.58 $^{\circ}C$, critical solution temp 147 $^{\circ}C$, Sidgwick et al. 1915)

22664 (shake flask-residue volume method, Booth & Everson 1948)

22000* (20 $^{\circ}C$, synthetic method/shake flask-optical, measured range 0–148 $^{\circ}C$, Ericksen & Dobbert 1955)

25000 (shake flask-spectrophotometry, Roberts et al. 1977)

2800 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)

23500, 58000 (20 $^{\circ}C$, 100 $^{\circ}C$, Verschueren 1977, 1983)

23790* (20.35 $^{\circ}C$, equilibrium cell-concn ratio-GC, measured range 20.35–139 $^{\circ}C$, Leet et al. 1987)

24125, 23194* (24.7, 25 $^{\circ}C$, calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)

46935, 54615, 58327 (75.9, 88.7, 98.5 $^{\circ}C$, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

19600 (shake flask-HPLC/UV at pH 4.45, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of the section):

- 20265* (149.5°C, mercury manometer, measured range 149.5–201.1°C, Goldblum et al. 1947)
 $\log(P/\text{mmHg}) = -2650/(T/K) + 8.457$; temp range 149.5–201.1°C (Hg manometer, Goldblum et al. 1947)
- 23.95* (extrapolated-regression of tabulated data, temp range 52–202.8°C, Stull 1947)
- 25.83 (calculated-Antoine eq., Dreisbach 1955)
 $\log(P/\text{mmHg}) = 7.53165 - 1875.3/(201.0 + t/^{\circ}\text{C})$, temp range: 110–240°C, (Antoine eq. for liquid state, Dreisbach 1955)
- 1333* (85.5°C, ebulliometry, measured range 85.5–202.1°C, Vonterres et al. 1955)
- 19.0 (gas saturation-diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
- 18.278* (24.90°C, gas saturation-diaphragm manometer, temp range 0–39°C, Biddiscombe & Martin 1958)
 $\log(P/\text{mmHg}) = 9.9653 - 3223.45/(t/^{\circ}\text{C} + 273)$; temp range 11–40°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
- $\log(P/\text{mmHg}) = 7.15904 - 1603.811/(t/^{\circ}\text{C} + 172.646)$; temp range 110–200°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; measurements, Andon et al. 1960)
- $\log(P/\text{mmHg}) = [-0.2185 \times 13483.8/(T/K)] + 9.135933$; temp range 52–202.8°C (Antoine eq., Weast 1972–73)
- 22.28 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log(P/\text{mmHg}) = 7.50798 - 1856.356/(199.065 + t/^{\circ}\text{C})$, temp range 149.5–201°C (Antoine eq. from reported exptl. data, Boublik et al. 1973)
- 4120* (114.99°C, diaphragm gauge, measured range 114.99–216.72 °C, Nasir et al. 1980)
- 5.33, 16.0 (20°C, 30°C, Verschuere 1977, 1983)
- 36.43 (calculated-Cox eq., Chao et al. 1983)
 $\log(P/\text{mmHg}) = [1 - 475.222/(T/K)] \times 10^{0.965085 - 6.89845 \times 10^{-4} \cdot (T/K) + 4.47100 \times 10^{-7} \cdot (T/K)^2}$; temp range: 278.05–705.85 K, (Cox eq., Chao et al. 1983)
- 22.1, 11.9 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.62485 - 1850.362/(198.462 + t/^{\circ}\text{C})$; temp range 149.5–201°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- $\log(P/\text{kPa}) = 6.28411 - 1580.594/(167.548 + t/^{\circ}\text{C})$; temp range 88.5–202.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 22.29 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.5080 - 1856.36/(199.07 + t/^{\circ}\text{C})$; temp range 150–201°C (Antoine eq., Dean 1985, 1992)
- 19.10 (Riddick et al. 1986)
- 79960* (466.35 K, vapor-liquid equilibrium, measured range 466.35–588.68 K, Klara et al. 1987)
- 19.08; 18.61 (interpolated-Antoine eq.-III, IV, Stephenson & Malanowski 1987)
 $\log(P_s/\text{kPa}) = 8.0462 - 2930.845/(T/K)$; temp range 273–285 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.28394 - 1603.811/(-100.504 + T/K)$; temp range 383–473 K, (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 9.0902 - 3223.45/(T/K)$; temp range 284–313 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 7.150 - 2123.548/(-59.018 + T/K)$; temp range 285–416 K (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.28579 - 1605.855/(-100.232 + T/K)$; temp range 410–477 K (Antoine eq.-V, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 5.80987 - 1293.277/(-135.465 + T/K)$; temp range 471–531 K (Antoine eq.-VI, liquid, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.64135 - 2069.208/(-26.534 + T/K)$, temp range: 523–633 K, (Antoine eq.-VII, liquid, Stephenson & Malanowski 1987)
- 19.70 (extrapolated-Antoine eq., Nesterova et al. 1990)
 $\log(P/\text{Pa}) = 64.02580 - 5272.296/(T/K) - 18.84252 \cdot \log(T/K) + 0.52858 \times 10^{-2} \cdot (T/K)$; temp range: 409–477 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
- $\log(P/\text{mmHg}) = 105.528 - 6.9748 \times 10^3/(T/K) - 35.083 \cdot \log(T/K) + 1.2508 \times 10^{-2} \cdot (T/K) - 2.4317 \times 10^{-12} \cdot (T/K)^2$; temp range 285–706 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0203, 0.0881 (8, 25°C , calculated, Leuenberger et al. 1985)
- 0.0875, 0.0627 (calculated-P/C, estimated-bond contribution, Meylan & Howard 1991)
- 0.0718 (computed-vapor-liquid equilibrium VLE data, Yaws et al. 1991)
- 0.1068 (calculated-P/C, Shiu et al. 1994)
- 0.0810, 0.0865* (24.7, 25°C , calculated-activity coeff. γ^∞ data, Dohnal & Fenclová 1995)
- 1.683, 2.990, 4.635 (75.9, 88.7, 98.5°C , vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
- 0.0848 (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)
- $\ln K_{\text{AW}} = 8.909 - 5722/(T/\text{K})$, temp range $20\text{--}100^\circ\text{C}$ (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
- 0.0868 (gas stripping-GC, Altschuh et al. 1999)
- 0.0641 (20°C , single equilibrium static technique SEST, Sheikheldin et al. 2001)
- 0.0765, 0.127* (20, 25°C , dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.96 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971; Hansch & Leo 1985)
- 2.02 (shake flask, Korenman et al. 1980)
- 1.94 (HPLC-RT correlation, Butte et al. 1981)
- 1.96 (generator column-HPLC, Wasik et al. 1981; Tewari et al. 1982)
- 1.96 (shake flask-UV, Saarikoski & Viluksela 1982)
- 1.98 (recommended, Sangster 1989, 1993)
- 1.96 (COMPUTOX databank, Kaiser 1993)
- 1.96 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

- 1.30 (golden ide, after 3 d, Freitag et al. 1985)
- 3.69 (algae, after 1 d, Freitag et al. 1985)
- 3.04 (activated sludge, after 5 d, Freitag et al. 1985)
- 1.03 (zebrafish, Butte et al. 1987)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.54 (Brookstone clay loam soil, Boyd 1982)
- 1.26 (calculated-S, Boyd 1982)
- 1.76 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct aqueous photolysis $k = 0.011 \pm 0.001 \text{ min}^{-1}$ with $t_{1/2} = 60.4 \text{ min}$ (Stegeman et al. 1993).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{NO}_3} = (7 \pm 1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of NO_3 radical with 2-methyl-2-butene (Japar & Niki 1975; Graham & Johnston 1978; Carter et al. 1981)

$k_{\text{OH}} = 48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of OH radical with 2-methyl-2-butene (Atkinson et al. 1979; Carter et al. 1981)

$k_{\text{NO}_3} = (8.10 \pm 1.16) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(300 \pm 1) \text{ K}$ with reference to the reaction of NO_3 radical with 2-methyl-2-butene (Carter et al. 1981; quoted, Atkinson 1991)

$k_{\text{O}_3} = (1.94 \pm 0.35) \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$; calculated tropospheric lifetimes of 60 d and 0.2 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

photooxidation half-life of 66–3480 h in water, based on reported reaction rate constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991)

$k = (1.3 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.5/2.0 (Hoigné & Bader 1983b)

$k_{\text{OH}} = 5.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = 1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = (9.20 \pm 2.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson et al. 1984)

$k_{\text{NO}_3} = (15.9 \pm 1.7) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $298 \pm 1 \text{ K}$ with reference to the reaction of NO_3 radical with phenol (Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{OH}}(\text{calc}) = 93.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{\text{OH}}(\text{exptl}) = 57 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 6.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (recommended, Atkinson 1989, 1990)

$k_{\text{NO}_3} = (9.74 \pm 0.74) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with reference to the reaction of NO_3 radical with 2-methyl-2-butene, and $k_{\text{OH}} = 64 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1992)

$k_{\text{OH}}(\text{calc}) = 34.42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}} = 5.2 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.22 \text{ d}$ under clear sky; $\tau = 0.19 \text{ d}$ under cloudy conditions at 298 K, reduced to 0.13 d due the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis:

Biodegradation: $t_{1/2} = 1\text{--}2 \text{ d}$ for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964)

completely degraded by a soil microflora within one day (Alexander & Lustigman 1966; quoted, Verschuuren 1983)

average rate $k = 55.0 \text{ mg COD g}^{-1} \cdot \text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2}(\text{aq. aerobic}) = 48\text{--}696 \text{ h}$, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);

$t_{1/2}(\text{aq. anaerobic}) = 360\text{--}1176 \text{ h}$, based on anaerobic screening test data (Horowitz et al. 1982; Shelton & Tiedje 1981; selected, Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 8.0 \text{ h}$, based on rate constant for the gas phase reaction with OH radical in air (Atkinson et al. 1979; quoted, Howard 1989);

photooxidation $t_{1/2} = 1.1\text{--}11.3 \text{ h}$ in air, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

calculated atmospheric lifetime $\tau = 0.22 \text{ d}$ under clear sky and $\tau = 0.19 \text{ d}$ under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to $\tau = 0.13 \text{ d}$ due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: $t_{1/2} = 48\text{--}696 \text{ h}$, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);

$k = (1.3 \pm 0.3) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.5/2.0 (Hoigné & Bader 1983);

photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reported reaction rate constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991).

Ground water: estimated half-life for cresols, $t_{1/2} = 0.01 \text{ yr}$ at Noordwijk (Zoeteman et al. 1981);

$t_{1/2} = 96\text{--}1176 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 48\text{--}696 \text{ h}$, based on unacclimated marine water grab sample data (Pfaender & Batholomew 1982; selected, Howard et al. 1991);

$t_{1/2} = 11.3 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 0.6 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.1.3.1
Reported aqueous solubilities of *m*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Leet et al. 1987		Dohnal & Fenclová1995	
shake flask-synthetic method		shake flask-optical method		equilibrium cell-conc ratio		vapor-liquid equil.-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
−0.20	22400	0	20000	20.35	23790	24.7	24125
24.7	23600	20	22000	40.05	25390	25	23194
47.0	26600	40	25000	58.45	30190	75.8	46935
61.9	30300	60	31000	77.25	37368	88.7	54615
74.5	35400	80	40000	98.15	49804	98.5	58327
87.5	42400	100	53000	119.75 ^a	78100		
116.9	65900	120	88000	138.95 ^b	143583		
139.4	119900	130	113000				
146.9	324000	140	156000	superscript a, at 204 kPa			
147.0	350700	142	170000	superscript b, at 366 kPa			
146.6	410600	144	189000				
140.5	612700	146	221000				
124.8	703200	147	264000				
109.3	804600	148	380000				
82.8	804600						
67.7	826000						
57.1	837000						
46.5	847900						
34.5	858500						
20.3	870500						
13.2	875800						

critical solution temp 147°C
mp/°C 4.0

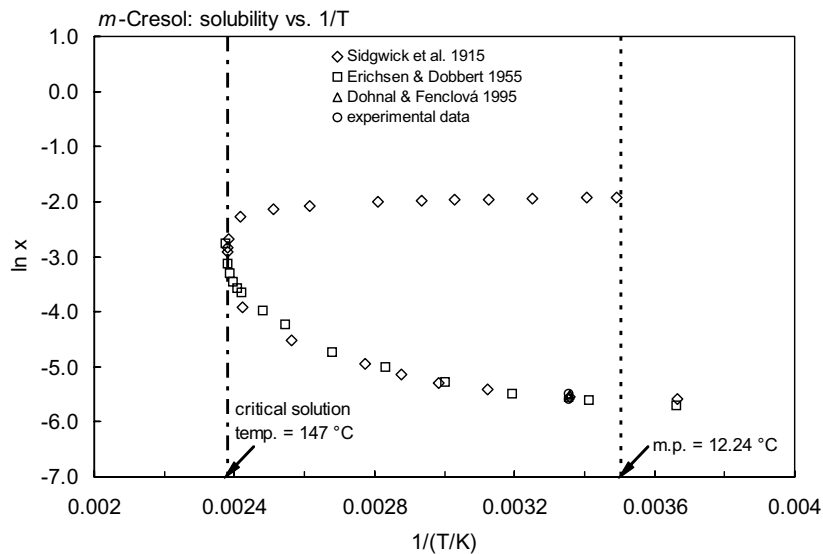


FIGURE 14.1.1.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for *m*-cresol.

TABLE 14.1.1.3.2

Reported vapor pressures of *m*-cresol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{llll} \log P = A - B/(T/K) & (1) & \ln P = A - B/(T/K) & (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) & P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P = A - B/(C + T/K) & (3) & & \\ \log P = A - B/(T/K) - C \cdot \log (T/K) & (4) & & \end{array}$$

1.

Stull 1947		Goldblum et al. 1947		Vonterres et al. 1955	
summary of literature data		static method-manometer		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
52.0	133.3	149.5	20265	85.5	1333
76.0	666.6	164.3	33464	105.2	3333
87.8	1333	172.0	42796	121.7	6666
101.4	2666	179.6	53862	131.6	9999
116.0	5333	187.4	67328	139.1	13332
125.8	7999	192.1	76927	150.0	19998
138.0	13332	196.3	86526	158.5	26664
157.3	26664	201.1	98925	163.1	33330
179.0	53329	149.6	20398	170.1	39997
202.8	101325	154.1	23731	173.0	43330
		176.4	48796	175.0	45553
mp/°C	10.8	183.4	60128	179.8	53329
		201.1	98925	183.5	66661
				189.8	73327
		eq. 1	P/mmHg	192.5	79993
		A	8.457	196.0	86659
		B	2650	198.8	93325
				202.1	101325

2.

Biddiscombe & Martin 1958				Nasir et al. 1980		Klara et al. 1987	
gas saturation		ebulliometry		diaphragm gauge		vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
			liquid				
0	2.00*	135.835	12174	114.99	4120	466.35	79960
4.90	2.933*	149.804	20418	121.25	5789	472.95	85540
7.20	4.533*	157.610	26762	127.46	7849	493.75	160600
9.15	4.40*	163.741	32816	133.4	10286	510.86	237900
11.0	5.866	169.814	39930	142.92	15223	531.35	366200
15.0	7.333	174.784	46538	156.29	25337	565.45	695500
17.65	9.866	179.331	53388	167.90	37430	588.68	1028500
19.80	11.47	182.979	59446	187.33	67950		
21.50	14.13	186.818	66415	203.4	106385	eq. 3	P/kPa
24.90	18.27	190.266	73225	216.72	149432	A	15.5337
26.95	27.73	193.424	79951			B	4594.0
29.75	30.80	196.418	86769			C	54.34
30.85	36.80	199.003	93024				

TABLE 14.1.1.3.2 (Continued)

Biddiscombe & Martin 1958				Nasir et al. 1980		Klara et al. 1987	
gas saturation		ebulliometry		diaphragm gauge		vapor-liquid equilibrium	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	T/K	P/Pa
33.25	43.20	199.694	94754				
39.10	57.60	200.250	96156				
	*solid	200.658	97201				
		201.216	98639				
bp/°C	202.231	201.557	99550				
		202.156	101118				
Antoine eq. for temp range:		202.737	102665				
11–40°C							
eq. 2	P/mmHg	Antoine eq. for temp range					
A	9.9653	110–200°C					
B	3223.45	eq. 2	P/mmHg				
C	273	A	7.15904				
		B	1603.811				
		C	172.646				
ΔH_v /(kJ mol ⁻¹)							
at bp	49.375						
at 25°C	61.714						

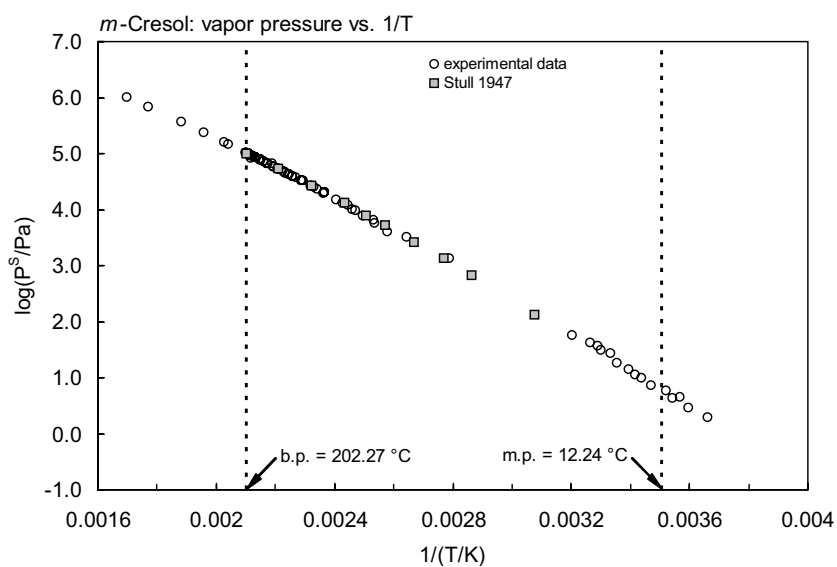
FIGURE 14.1.1.3.2 Logarithm of vapor pressure versus reciprocal temperature for *m*-cresol.

TABLE 14.1.1.3.3

Reported Henry's law constants of *m*-cresol at various temperatures and temperature dependence equations

$$\begin{aligned} \ln K_{AW} &= A - B/(T/K) & (1) & \log K_{AW} = A - B/(T/K) & (1a) \\ \ln (1/K_{AW}) &= A - B/(T/K) & (2) & \log (1/K_{AW}) = A - B/(T/K) & (2a) \\ \ln (k_H/\text{atm}) &= A - B/(T/K) & (3) & & \\ \ln H &= A - B/(T/K) & (4) & \log H = A - B/(T/K) & (4a) \\ K_{AW} &= A - B \cdot (T/K) + C \cdot (T/K)^2 & (5) & & \end{aligned}$$

Dohnal & Fenclová 1995		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-GC/MS	
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)
24.7	0.0810*	278.15	0.0148
25.0	0.0865*	278.25	0.0192
75.9	1.683	283.15	0.0283
88.7	2.990	283.25	0.0378
98.5	4.635	283.25	0.0272
25.0	0.0848#	283.25	0.0293
25.0	0.0846\$	288.15	0.0444
		288.25	0.0450
#calculated from eq. 1		293.15	0.0976
\$calculated from eq. 3		293.15	0.0682
*data from literature		293.15	0.0723
		293.15	0.0786
eq. 1	K _{AW}	293.15	0.0771
A	8.909	293.15	0.0976
B	5722	293.25	0.0901
		293.15	0.0810
enthalpy of hydration:		298.15	0.1306
ΔH _K /(kJ mol ⁻¹) = 47.6 ± 0.5		298.15	0.1252
OR		293	0.0765
eq. 3	k _H /kPa	298	0.1270
A	21.650		
B	5994		
ΔH _K /(kJ mol ⁻¹) = 49.8 ± 0.6			

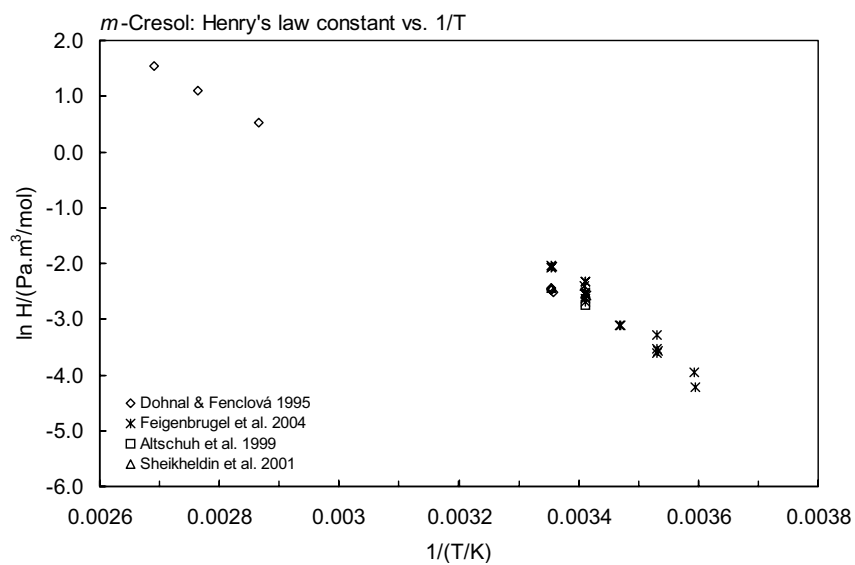
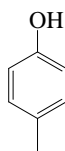


FIGURE 14.1.1.3.3 Logarithm of Henry's law constant versus reciprocal temperature for *m*-cresol.

14.1.1.4 *p*-Cresol

Common Name: *p*-Cresol

Synonym: *p*-cresylic acid, 1-hydroxy-4-methylbenzene, 4-hydroxytoluene, 4-methylphenol, *p*-hydroxytoluene, *p*-methylphenol, 4-cresol

Chemical Name: 4-methylphenol

CAS Registry No: 106-44-5

Molecular Formula: C_7H_8O , $CH_3C_6H_4OH$

Molecular Weight: 108.138

Melting Point ($^{\circ}C$):

34.77 (Lide 2003)

Boiling Point ($^{\circ}C$):

201.98 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0178 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

10.26 (Pearce & Simkins 1968, Dean 1985, Riddick et al. 1986; Howard 1989)

10.28 (Serjeant & Dempsey 1979; Tratnyek & Hoigné 1991; Haderlein & Schwarzenbach 1993)

10.17 (Weast 1982–83)

Molar Volume (cm^3/mol):

125.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.53 (at normal bp, Biddiscombe & Martin 1958)

47.55 (at normal boiling point, Andon et al. 1960)

43.2 (Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

73.93 (at $25^{\circ}C$, Biddiscombe & Martin 1958; Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

12.72 (Tsonopoulos & Prausnitz 1971; Dean 1992)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

53.22 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.802 (mp at $34.77^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

22400* ($40.2^{\circ}C$, shake flask, measured range 40.2 – $143.5^{\circ}C$, critical solution temp $143.5^{\circ}C$, Sidgwaick et al. 1915)

24230 (shake flask-residue volume method, Booth & Everson 1948)

19000 (shake -flask-UV, Blackman et al. 1955)

17000* ($20^{\circ}C$, synthetic method/shake flask-optical, measured range 0 – $143.7^{\circ}C$, Ericksen & Dobbert 1955)

21000 (shake flask-spectrophotometry, Roberts et al. 1977)

24000, 53000 ($40^{\circ}C$, $100^{\circ}C$, Verschueren 1977, 1983)

21500* (calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)

43534, 50064, 54615 (75.9 , 88.7 , $98.5^{\circ}C$, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

22000 (shake flask-HPLC/UV at pH 3.9, Varhaníčkova et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

17599* ($145.7^{\circ}C$, mercury manometer, measured range 145.7 – $200.8^{\circ}C$, Goldblum et al. 1947)

- $\log (P/\text{mmHg}) = -2680/(T/K) + 8.524$; temp range 145.7–200.9°C (Hg manometer, Goldblum et al. 1947)
 21.89* (extrapolated-regression of tabulated data, temp range 53–201.8°C, Stull 1947)
 7605* (128.65 °C, ebulliometry, measured range 128.65–201.88 °C, Dreisbach & Shrader 1949)
 26.34 (calculated-Antoine eq., Dreisbach 1955)
 $\log (P/\text{mmHg}) = 7.52971 - 1872.4/(201.0 + t/^{\circ}\text{C})$; temp range 97–250°C (Antoine eq. for liquid state, Dreisbach 1955)
 15.91 (gas saturation-diaphragm manometer fitted to Antoine eq., Biddiscombe & Martin 1958)
 12.93* (23.35°C, gas saturation-diaphragm manometer, measured range 0–34.15°C, Biddiscombe & Martin 1958)
 $\log (P/\text{mmHg}) = 12.0298 - 3861.98/(t/^{\circ}\text{C} + 273)$; temp range 0–34°C (Antoine eq. from gas-saturation and diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 $\log (P/\text{mmHg}) = 7.11767 - 1566.029/(t/^{\circ}\text{C} + 167.680)$; temp range 110–200°C (Antoine eq. from gas-saturation-diaphragm manometer methods, Biddiscombe & Martin. 1958; Andon et al. 1960)
 133.3 (53°C, Andon et al. 1960; Haque et al. 1980)
 $\log (P/\text{mmHg}) = [-0.2185 \times 13611.7/(T/K)] + 9.190555$; temp range 53–201.8°C (Antoine eq., Weast 1972–73)
 11.8 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.03508 - 1511.08/(161.854 + t/^{\circ}\text{C})$; temp range 128–210.88°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1973)
 13.94 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 475.109/(T/K)] \times 10^{\{1.07944 - 11.6938 \times 10^{-4} \cdot (T/K) + 9.28202 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 323.20–704.65 K, (Cox eq., Chao et al. 1983)
 11.8, 17.5 (calculated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.15637 - 1508.694/(161.594 + t/^{\circ}\text{C})$, temp range 128–201.9°C (Antoine eq. from reported exptl. data of Dreisbach & Shrader 1949, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.44531 - 1713.242/(183.846 + t/^{\circ}\text{C})$; temp range 15.7–200.9°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 11.83 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.03508 - 1511.08/(161.85 + t/^{\circ}\text{C})$; temp range 128–202°C (Antoine eq., Dean 1985, 1992)
 17.3 (Riddick et al. 1986)
 15.6 (calculated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 12.098 - 3861.98/(T/K)$; temp range 273–307 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.16859 - 3868.314/(T/K)$; temp range 277–307 K (Antoine eq.-II, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.24257 - 1566.029/(-105.47 + T/K)$; temp range 383–473 K (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.83697 - 1930.688/(-73.422 + T/K)$; temp range 308–393 K (Antoine eq.-IV, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 5.2376 - 1563.08/(-105.776 + T/K)$; temp range 385–477 K (Antoine eq.-V, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19164 - 1533.535/(-108.781 + T/K)$; temp range 463–533 K (Antoine eq.-VI, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.99685 - 2310.405/(-10.362 + T/K)$; temp range 523–635 K (Antoine eq.-VII, Stephenson & Malanowski 1987)
 16.1 (extrapolated-Antoine eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 93.42570 - 6409.054/(T/K) - 29.82622 \cdot \log (T/K) + 1.03314 \times 10^{-2} \cdot (T/K)$; temp range: 397–476 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe & Martin 1958, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 122.8998 - 7.6175 \times 10^3/(T/K) - 41.637 \cdot \log (T/K) + 1.5709 \times 10^{-2} \cdot (T/K) - 8.9199 \times 10^{-13} \cdot (T/K)^2$; temp range 308–705 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0802; 0.0699; 1.0820 (exptl., calculated-group contribution; calculated-bond contribution Hine & Mookerjee 1975)

0.0223, 0.0973 (8, 25°C, calculated, Leuenberger et al. 1985)
 0.689 (calculated-P/C, Neely & Blau 1985)
 0.0397 (calculated-VLE vapor liquid equilibrium data, Yaws et al. 1991)
 0.0653 (calculated-P/C, Shiu et al. 1994)
 0.0783*, 0.297 (25, 40.2°C, calculated-activity coeff. γ^∞ data, Dohnal & Fenclová 1995)
 1.735, 3.144, 4.774 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.0801 (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 9.328 - 5865/(T/K)$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 < 0.347 (gas stripping-GC, Altschuh et al. 1999)
 0.102 (calculated-group contribution, Lee et al. 2000)
 0.0582, 0.0989* (20, 25°C, dynamic equilibrium system/gas stripping-GC/MS, Feigenbrugel et al. 2004)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.94 (shake flask-UV, Fujita et al. 1964)
 1.92, 1.94, 1.95 (quoted literature values, Leo et al. 1971; Hansch & Leo 1979, Hansch & Leo 1985)
 1.99 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
 1.94 (LC- k' correlation, Carlson et al. 1975)
 2.17 (shake flask, Korenman et al. 1980)
 1.97 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.92, 1.98 ± 0.07 (selected best lit. value, exptl.-ALPM, Garst & Wilson 1984)
 1.62 (HPLC- k' correlation, Haky & Young 1984)
 1.73 (calculated-activity coeff. γ from UNIFAC, Campbell & Luthy 1985)
 1.91 (HPLC- k' correlation, Miyake et al. 1987)
 1.94 (RP-HPLC-capacity ratio, Minick et al. 1988)
 1.94 (recommended, Hansch et al. 1995)
 1.90; 2.06, 2.12, 1.94 (solid-phase microextraction; calculated- K_{OW} program, calculated-CLOGP, quoted exptl., Dean et al. 1996)
 1.53, 1.53, 1.69, 1.76 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.26 (estimated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

2.81 (Coyote Creek sediment, Smith et al. 1978)
 1.69 (Brookstone clayloam soil, Boyd 1982)
 -0.046 (predicted-S, Boyd 1982)
 1.76 (calculated- K_{OW} , Kollig 1993)
 2.70 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.15, 2.33 (soils: organic carbon $OC \geq 0.1\%$ and pH 2.0–7.4, $OC \geq 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 167$ d, estimated from a lake as calculated from equations of Mackay & Wolkoff 1973 (Smith et al. 1978).

Photolysis:

$k = 6.8 \times 10^{-7} \text{ s}^{-1}$ under overcast weather of April at 25°C; $t_{1/2} \sim 4800$ h in river, $t_{1/2} > 10000$ h in both eutrophic lake and pond and $t_{1/2} = 2400$ h in oligotrophic lake, based on an average photolysis rate on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978; quoted, Howard 1989)
 photolytic $t_{1/2} = 5800$ h in aquatics (Haque et al. 1980).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 144\text{--}11325$ h in water, based on measured rate data for reactions with singlet oxygen and hydroxyl radical in aqueous solution (Anbar & Neta 1967; Scully & Hoigne 1987; quoted, Howard et al. 1991)

$k_{\text{NO}_3} = (13 \pm 2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 ± 1 K (Japar & Niki 1975; Graham & Johnston 1978; quoted, Carter et al. 1981)

$k(\text{aq.}) = 20 \text{ M}^{-1} \text{ s}^{-1}$, averaged over 24-h day (Smith et al. 1978)

$k_{\text{OH}} = 38 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 ± 1 K (Atkinson et al. 1979; quoted, Carter et al. 1981)

photooxidation $t_{1/2} = 10$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson et al. 1979; quoted, Howard 1989)

$k_{\text{NO}_3} = (15 \pm 2.4) \times 10^{-12} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 300 ± 1 K in air (relative rate technique with reference to 2-methyl-2-butene, Carter et al. 1981; quoted, Atkinson 1991)

$k_{\text{O}_3} = (4.71 \pm 0.66) \times 10^{-19} \text{ cm}^3 \cdot \text{molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K; calculated tropospheric lifetimes of 25 d and 0.3 d due to reaction with O_3 and OH radical, respectively, at room temp. (Atkinson et al. 1982, 1984; Atkinson 1985)

$k = (3.0 \pm 0.6) \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water at pH 1.5/2.0 (Hoigné & Bader 1983b)

$k_{\text{OH}} = 4.50 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{NO}_3} = 1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson & Lloyd 1984; quoted, Carlier et al. 1986)

$k_{\text{OH}} = (16.6 \pm 1.8) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 ± 1 K (relative technique with reference to *m*-cresol, Atkinson et al. 1984; quoted, Atkinson 1991)

$k_{\text{NO}_3} = (1.27 \pm 0.36) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K in air (Atkinson et al. 1984)

photooxidation $t_{1/2} = 1.5\text{--}15$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Atkinson 1985; selected, Howard et al. 1991)

$k_{\text{OH}}(\text{exptl}) = 44.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{obs.}) = 41 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 56.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{exptl}) = 42 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1985; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{\text{OH}}(\text{calc}) = 44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{exptl}) = 44 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR, Atkinson 1987; quoted, Sabljic & Güesten 1990)

$k = 1.1 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8.3, $2.4 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8.8, $1.6 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 10, $3.5 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 11.5 for the reaction with singlet oxygen in water at $(19 \pm 2)^\circ\text{C}$ (Scully & Hoigné 1987)

$k_{\text{NO}_3} = 21.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al. 1988; quoted, Sabljic & Güesten 1990; Müller & Klein 1991)

$k_{\text{OH}} = 4.7 \times 10^{-1} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989, 1990)

$k = (9.6 \pm 2.8) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $(27 \pm 1)^\circ\text{C}$ (Tratnyek & Hoigné 1991)

$k_{\text{NO}_3} = (10.7 \pm 1) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 ± 2 K, $k_{\text{OH}} = 47 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson et al. 1992)

$k_{\text{OH}}(\text{calc}) = 30.83 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{\text{OH}} = 5.2 \times 10^{-11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, and $k_{\text{OH}}(\text{aq.}) = 1.2 \times 10^{-10} \text{ M}^{-1} \text{ s}^{-1}$, the calculated atmospheric lifetime $\tau = 0.23$ d under clear sky; $\tau = 0.18$ d under cloudy conditions at 298 K, reduced to 0.11 d due to the average temperature of tropospheric clouds at 283 K (Feigenbrugel et al. 2004)

Hydrolysis: no hydrolyzable functional groups (Smith et al. 1978).

Biodegradation: $t_{1/2} = 1\text{--}2$ d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964)

Completely degraded by a soil microflora in one day (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate $k = 55.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2} = 12$ h in eutrophic lake for a point source continuously discharging $1.0 \text{ }\mu\text{g/mL}$ predicted by one compartment model for all processes including dilution (Smith et al. 1978); laboratory determined $k = 5.2 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ at 25°C (Smith et al. 1978)

$k(\text{calc}) = 1.7 \text{ d}^{-1}$ in river water, $k = 0.8\text{--}4.7 \text{ d}^{-1}$ in estuary water and $k = 2.8\text{--}4.8 \text{ d}^{-1}$ in marine water after a lag period (Vashon & Schwab 1982; quoted, Battersby 1990);

$t_{1/2}(\text{aq. aerobic}) = 1\text{--}16$ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; selected, Howard et al. 1991)

$t_{1/2}(\text{aq. anaerobic}) = 240\text{--}672$ h, based on anaerobic screening test data (Boyd et al. 1983; Horowitz et al. 1982; selected, Howard et al. 1991);

$k = 1.72 \times 10^{-17}$ mol cell⁻¹ h⁻¹ in pure culture system (Banerjee et al. 1984).

Biotransformation: estimated $t_{1/2} = 12$ h in river, eutrophic lake and pond and $t_{1/2} > 10000$ h in oligotrophic lake, based on an average photolysis rate on a summer day at 40°N latitude by the one compartment model (Smith et al. 1978).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 10$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson et al. 1979; quoted, Howard 1989);

photooxidation $t_{1/2} = 1.5\text{--}15$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Atkinson 1985; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 d (Kelly et al. 1994).

calculated atmospheric lifetime $\tau = 0.23$ d under clear sky and $\tau = 0.18$ d under cloudy conditions based on reactions with OH radical in gas and aqueous phases at 298 K, reduced to $\tau = 0.11$ d due to average temperature of tropospheric cloud at 283 K (Feigenbrugel et al. 2004)

Surface water: $t_{1/2} = 0.55$ h in river, $t_{1/2} = 12$ h in pond and eutrophic lake, and $t_{1/2} = 2400$ h in oligotrophic lake for a point source continuously discharging 1.0 µg/mL predicted by one compartment model for all processes including dilution (Smith et al. 1978; quoted, Howard 1989);

rate constant $k = (3.0 \pm 0.6) \times 10^4$ M⁻¹·s⁻¹ for the reaction with ozone at pH 1.5/2.0 in water (Hoigné & Bader 1983b);

$t_{1/2} = 1\text{--}16$ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{1/2} = 500$ h for the reaction with singlet oxygen in water at pH 8 and $(19 \pm 2)^\circ\text{C}$ (Scully & Hoigné 1987).

Ground water: estimated half-life for cresols, $t_{1/2} = 0.01$ yr at Noordwijk (Zoeteman et al. 1981); $t_{1/2} = 2\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil:

$t_{1/2} = 1\text{--}16$ h, based on unacclimated marine and freshwater grab sample data (Van Veld & Spain 1983; Rogers et al. 1984; quoted, Howard et al. 1991);

$t_{1/2} = 0.5$ d in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 1.0$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.1.4.1
Reported aqueous solubilities of *p*-cresol at various temperatures

Sidgwick et al. 1915		Erichsen & Dobbert 1955		Dohnal & Fenclová 1995	
shake flask-synthetic method		shake flask-optical method		vapor-liquid equil.-UV	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
40.2	22400	0	10000	25	21500
52.6	24900	20	17000	40.2	22840
63.5	28000	40	23000	75.9	43534
73.5	31900	60	30000	88.7	50064
84.0	37200	80	37000	98.5	54615
88.8	40600	100	48000	100	56146
94.0	44700	110	56000		
124.5	74200	120	72000		
139.4	151000	130	101000		
141.2	200700	140	177000		
143.5	301300	142	226000		
143.4	400800	143	264000		
141.5	506300	143.5	340000		
134.8	606100	148	380000		
111.6	719100				
77.9	704000				
37.4	836100				
27.5	844800				
17.2	852800				
8.7	868600				
9.2	879000				
10.8	900900				
17.1	946800				
20.3	960100				
24.0	922700				
27.5	983200				
29.9	990600				
33.8	1000000				
critical solution temp 143.5°C					
triple point 8.7°C					

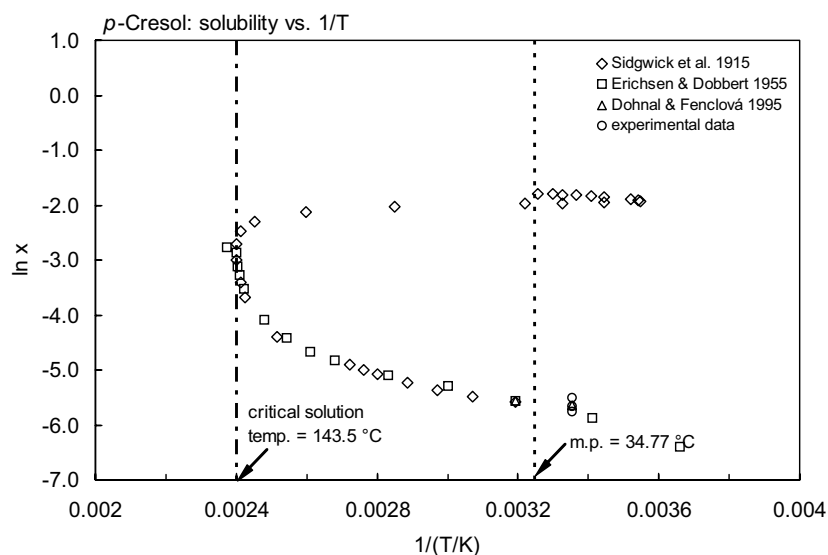


FIGURE 14.1.1.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for *p*-cresol.

TABLE 14.1.1.4.2

Reported vapor pressures of *p*-cresol at various temperatures and the coefficients for the vapor pressure equations

$$\begin{array}{ll} \log P = A - B/(T/K) & (1) \quad \ln P = A - B/(T/K) \quad (1a) \\ \log P = A - B/(C + t/^{\circ}\text{C}) & (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a) \\ \log P = A - B/(C + T/K) & (3) \\ \log P = A - B/(T/K) - C \cdot \log(T/K) & (4) \end{array}$$

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
							solid		liquid
53.0	133.3	145.7	17599	128.65	7605	0	1.493	124.151	7518
76.5	666.6	163.6	32664	131.26	10114	4.75	1.640	138.025	13204
88.6	1333	171.6	42263	143.86	16500	8.60	2.653	145.593	17517
102.3	2666	179.2	53329	171.27	42066	10.8	4.066	155.395	24845
117.7	5333	187.2	67194	187.17	67661	13.9	4.880	162.723	31824
127.0	7999	193.7	80660	201.88	101325	16.8	7.199	168.937	38934
140.0	13332	200.8	98392			20.0	9.013	173.819	45366
157.7	26664	153.0	22931			22.0	12.08	178.598	52497
179.4	53329	183.8	61062	bp/°C	201.88	23.35	13.00	183.663	60995
201.8	101325	190.8	74261			28.85	21.86	186.521	66259
		197.1	88526			29.75	25.60	190.578	74355
mp/°C	35.5	200.8	98392			32.55	31.60	192.90	79336
						34.15	38.53	193.029	79631
		eq. 1	P/mmHg					197.102	89029
		A	8.308					198.609	92732
		B	2520			bp/°C	201.94	199.666	95395
								200.226	96828
						for temp range:		200.535	97964
						0–34°C		201.122	99164
						eq. 2	P/mmHg	201.719	100728
						A	12.0298	202.269	102205

TABLE 14.1.1.4.2 (Continued)

Stull 1947		Goldblum et al. 1947		Dreisbach & S. 1949		Biddiscombe & Martin 1958			
summary of lit. data		mercury manometer		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
						B	3861.98	202.985	104133
						C	273		
						$\Delta H_v/(\text{kJ mol}^{-1})$		for temp range:	
						at bp	49.534	110–200°C	
						at 25°C	73.931	eq. 2	P/mmHg
								A	7.11767
								B	1566.029
								C	167.680

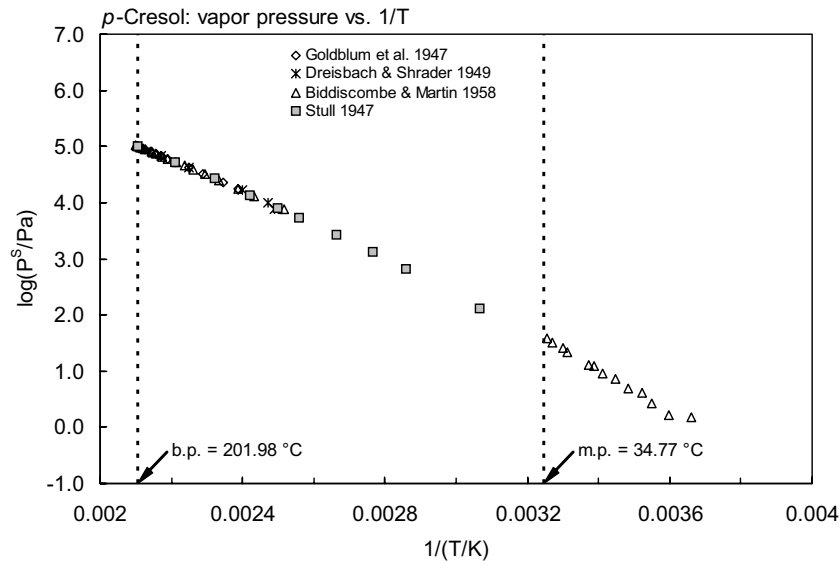


FIGURE 14.1.1.4.2 Logarithm of vapor pressure versus reciprocal temperature for *p*-cresol.

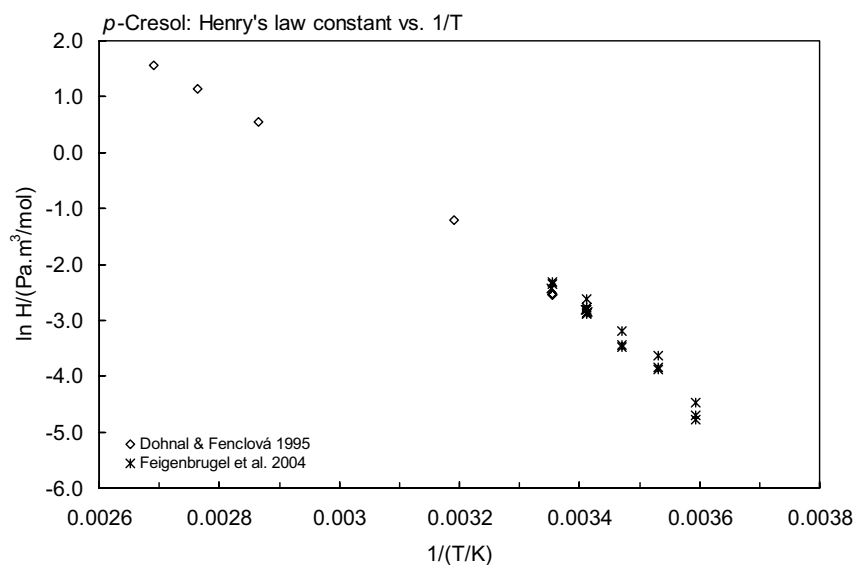
TABLE 14.1.1.4.3
Reported Henry's law constants of *m*-cresol at various temperatures and temperature dependence equations

$\ln K_{AW} = A - B/(T/K)$		(1)	$\log K_{AW} = A - B/(T/K)$		(1a)
$\ln (1/K_{AW}) = A - B/(T/K)$		(2)	$\log (1/K_{AW}) = A - B/(T/K)$		(2a)
$\ln (k_H/\text{atm}) = A - B/(T/K)$		(3)			
$\ln H = A - B/(T/K)$		(4)	$\log H = A - B/(T/K)$		(4a)
$K_{AW} = A - B \cdot (T/K) + C \cdot (T/K)^2$		(5)			
Dohnal & Fenclová 1995		Feigenbrugel et al. 2004			
vapor-liquid equilibrium		gas stripping-GC/MS			
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)		
25.0	0.0783*	278.25	0.00914		
40.2	0.297*	278.25	0.01148		
75.9	1.735	278.35	0.00846		

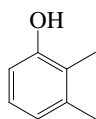
(Continued)

TABLE 14.1.1.4.3 (Continued)

Dohnal & Fenclová 1995		Feigenbrugel et al. 2004	
vapor-liquid equilibrium		gas stripping-GC/MS	
t/°C	H/(Pa m ³ /mol)	T/K	H/(Pa m ³ /mol)
88.7	3.144	283.15	0.0262
98.5	4.774	283.15	0.0215
25.0	0.0801#	283.25	0.0207
25.0	0.0792\$	288.10	0.0323
		288.15	0.0414
#calculated from eq. 1		288.20	0.0307
\$calculated from eq. 3		293.10	0.0557
*data from literature		293.15	0.0724
		293.15	0.0627
eq. 1	K _{AW}	293.15	0.0606
A	9.328	293.15	0.0563
B	5865	293.25	0.0602
		298.15	0.0943
enthalpy of hydration:		298.25	0.0875
$\Delta H_K/(\text{kJ mol}^{-1}) = 48.8 \pm 0.6$		293	0.0582
OR		298	0.0989
eq. 3	k _H /kPa		
A	22.071		
B	6138		
$\Delta H_K/(\text{kJ mol}^{-1}) = 51.0 \pm 0.6$			

FIGURE 14.1.1.4.3 Logarithm of Henry's law constant versus reciprocal temperature for *p*-cresol.

14.1.1.5 2,3-Dimethylphenol



Common Name: 2,3-Dimethylphenol

Synonym: 2,3-xylenol, 1-hydroxy-2,3-dimethylbenzene

Chemical Name: 2,3-dimethylphenol

CAS Registry No: 526-75-0

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

72.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

216.9 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.54 (Dohnal & Fenclová 1995)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.08, 47.32 ($25^{\circ}C$, normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.342$ (mp at $72.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

40000* ($150^{\circ}C$, shake flask-optical method, measured range 150 – $208.8^{\circ}C$, Erichsen & Dobbert 1955)

3930 ($20^{\circ}C$, shake flask or batch contacting technique-UV, Dohnal & Fenclová 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

133.3* ($56^{\circ}C$, summary of literature data, temp range 56 – $219.0^{\circ}C$, Stull 1947)

1333* ($84.0^{\circ}C$, ebulliometry, measured range 84.0 – $219.0^{\circ}C$, Vonterres et al. 1955)

3.64* ($24.71^{\circ}C$, ebulliometry/gas saturation, measured range 10 – $45^{\circ}C$, Andon et al. 1960)

$\log(P/mmHg) = 13.1606 - 4389.99/(t/^{\circ}C + 273)$; temp range 10 – $50^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 7.04268 - 1069.164/(t/^{\circ}C + 169.744)$; temp range 149 – $219^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/kPa) = 6.13887 - 1588.200/(167.385 + t/^{\circ}C)$; temp range 149 – $218^{\circ}C$ (Antoine eq. derived from experimental data of Andon et al. 1960, Boublik et al. 1984)

$\log(P/kPa) = 6.01592 - 1644.433/(192.286 + t/^{\circ}C)$, temp range 84 – $219^{\circ}C$ (Antoine eq. derived from experimental data of Vonterres et al. 1955, Boublik et al. 1984)

$\log(P_s/kPa) = 12.29616 - 4394.694/(T/K)$; temp range 282 – $323\ K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.17998 - 1619.086/(-102.197 + T/K)$; temp range 433 – $492\ K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 82.92733 - 6.0367 \times 10^3/(T/K) - 26.948 \cdot \log(T/K) + 9.739 \times 10^{-3} \cdot (T/K) + 2.5196 \times 10^{-12} \cdot (T/K)^2$; temp range 346 – $723\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

0.0631, 0.0952 (20 , $25^{\circ}C$, calculated-limiting activity coefficient γ^{∞} data, Dohnal & Fenclová 1995)

2.96, 5.656, 8.652 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

$\ln K_{AW} = 11.858 - 6567/(T/K)$; temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.48 (HPLC-RT correlation, Makovskaya et al. 1995b)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Half-Lives in the Environment:

TABLE 14.1.1.5.1

Reported aqueous solubilities of 2,3-dimethylphenol at various temperatures

Erichsen & Dobbett 1955

shake flask-optical method

$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
150	40000
160	48000
170	58000
180	70000
190	94000
200	140000
202	156000
204	175000
206	200000
208	252000
208.8	365000

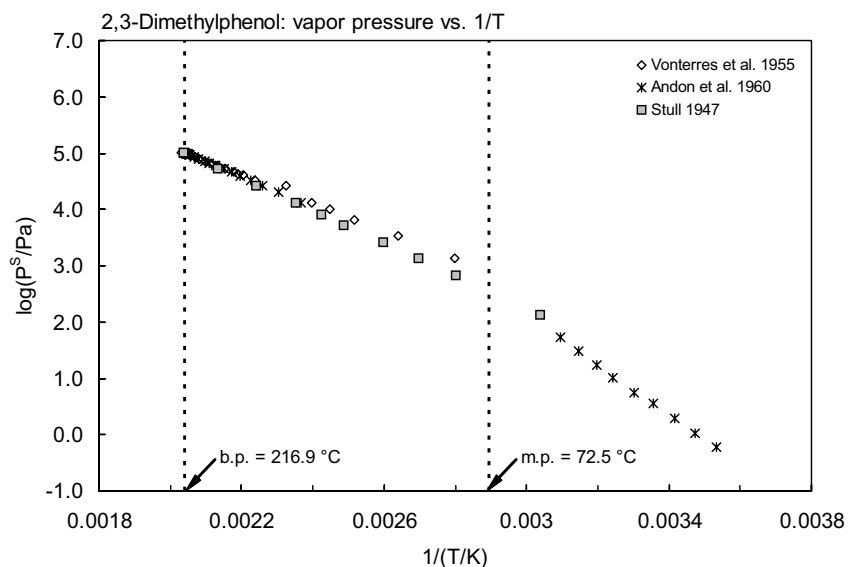


FIGURE 14.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,3-dimethylphenol.

TABLE 14.1.1.5.2

Reported vapor pressures of 2,3-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2)$$

$$\ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

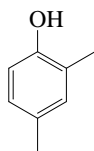
Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
56.0	133	84.0	1333	9.91	0.609	149.346	13304
83.8	666.6	105.6	3333	14.70	1.072	160.94	20045
97.6	1333	124.0	6666	19.70	1.933	169.634	26704
112.0	2666	135.2	9999	24.71	3.640	176.314	32963
129.2	5333	144.0	13332	29.58	5.650	182.500	39779
139.5	7999	157.0	26664	35.19	10.13	187.374	45920
152.2	13332	174.0	33330	39.54	17.33	192.094	53573
173.0	26664	180.2	39997	44.81	29.86	196.778	59919
196.0	53329	183.6	43330	49.88	52.93	200.752	66779
218.0	101325	186.1	46663			204.000	72842
		191.0	53329	mp/°C	72.57	207.54	79951
mp/°C	75.0	196.0	59995	bp/°C	216.87	210.672	86542
		200.0	66661			213.454	93026
		203.9	73327	for temp range:		214.137	94644
		207.0	79993	9–50°C		214.788	96151
		210.1	86659	eq. 2	P/mmHg	215.091	96929
		213.5	93325	A	13.1606	215.646	98283
		219.0	101325	B	4389.06	216.144	99513
				C	273	216.987	101613
						217.323	102400

(Continued)

TABLE 14.1.1.5.2 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				$\Delta H_v/(\text{kJ mol}^{-1})$		217.928	104010
				at 25°C	84.015		
				at bp	47.32	for temp range:	
						149–218°C	
						eq. 2	P/mmHg
						A	7.04268
						B	1609.184
						C	169.774

14.1.1.6 2,4-Dimethylphenol



Common Name: 2,4-Dimethylphenol

Synonym: 2,4-xylenol, *as-m*-xylenol, 1-hydroxy-2,4-dimethylbenzene

Chemical Name: 2,4-dimethylphenol

CAS Registry No: 105-67-9

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

24.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

210.98 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0202 (Andon et al. 1960)

0.9650 (Weast 1982–83)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.60 (Herington & Kynaston 1957; quoted, Callahan et al. 1979)

10.58 (Dean 1985)

10.63 (Riddick et al. 1986; Howard 1989)

10.10 (Kollig 1993)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

47.15 (at normal boiling point, Andon et al. 1960)

65.86 (at $25^{\circ}C$, Andon et al. 1960; Dean 1992)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

8795 (shake flask-UV at pH 5.1, Blackman et al. 1955)

6200 (shake flask-UV at pH 6.5, Blackman et al. 1955)

6200* (synthetic method/shake flask-optical, extrapolated value, measured range 160 – $213.5^{\circ}C$, Ericksen & Dobbert 1955)

7868 (shake flask-LSC, Banerjee et al. 1980)

7888 (shake flask-radioactive analysis, Veith et al. 1980)

7819 (generator column-HPLC, Wasik et al. 1981)

4200 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

7929 (calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)

8200 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($51.8^{\circ}C$, summary of literature data, temp range 51.8 – $211.0^{\circ}C$, Stull 1947)

21.78 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.37688 - 1838.9/(1999.0 + t/^{\circ}C)$; temp range 115 – $245^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

- 1333* (89.50 °C, ebulliometry, measured range 89.50–211.0 °C, Vonterres et al. 1955)
 12.81* (24.87°C, ebulliometric and gas-saturation methods, measured range 9–45°C Andon et al. 1960)
 13.02 (interpolated-Antoine eq. derived from exptl. results, Andon et al. 1960)
 $\log (P/\text{mmHg}) = 10.5277 - 3439.99/(t/^{\circ}\text{C} + 273)$; temp range 9–45°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
 $\log (P/\text{mmHg}) = 7.04694 - 1581.391/(t/^{\circ}\text{C} + 168.652)$; temp range 114–212°C (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
 $\log (P/\text{mmHg}) = [-0.2185 \times 13130.2/(T/K)] + 8.867260$; temp range 51.8–211.5°C (Antoine eq., Weast 1972–73)
 10.28 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.05539 - 1587.459/(169.339 + t/^{\circ}\text{C})$; temp range 144.4–212.3°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
 13.17 (calculated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 483.876/(T/K)] \times 10^{\{0.999891 - 8.94506 \times 10^{-4} \cdot (T/K) + 6.96026 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 298.02–707.95 K, (Cox eq., Chao et al. 1983)
 10.29, 20.22 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.18152 - 1588.34/(169.437 + t/^{\circ}\text{C})$, temp range 144.4–212.3°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 7.02271 - 2183.475/(225.488 + t/^{\circ}\text{C})$; temp range 89.5–211°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
 10.28 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.05539 - 1587.46/(169.34 + t/^{\circ}\text{C})$; temp range 144–212°C (Antoine eq., Dean 1985, 1992)
 12.87 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 9.65613 - 3442.574/(T/K)$; temp range 282–318 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.1672 - 1578.685/(-104.772 + T/K)$; temp range 429–486 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 12.96 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 86.11491 - 6138.775/(T/K) - 27.12977 \cdot \log (T/K) + 0.91169 \times 10^{-2} \cdot (T/K)$; temp range 418–485 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1960, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 53.3866 - 5.1516 \times 10^3/(T/K) - 15.095 \cdot \log (T/K) - 1.3196 \times 10^{-9} \cdot (T/K) + 2.8455 \times 10^{-6} \cdot (T/K)^2$; temp range 346–708 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.722 (calculate-P/C, Mabey et al. 1982)
 500 (EPICS-GC, Ashworth et al. 1988)
 500* (EPICS-GC/FID, measured range 10–30°C, Ashworth et al. 1988)
 $\ln [H/(\text{atm m}^3/\text{mol})] = -16.34 - 3307/(T/K)$, temp range 10–30°C (EPICS measurements, Ashworth et al. 1988)
 0.0638 (8°C, Leuenberger et al. 1985)
 0.203, 0.0692 (calculated-P/C, estimated-bond contribution, Meylan & Howard 1991)
 0.1815 (calculated-P/C, Shiu et al. 1994)
 0.199* (calculated-limiting activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)
 4.338, 7.491, 11.46 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.202* (extrapolated-vapor liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 10.077 - 5811/(T/K)$; temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 0.154 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)
 643 (20°C, selected from literature experimentally measured data - poor correlation coefficient, Staudinger & Roberts 2001)
 $\log K_{AW} = -5.192 + 1563/(T/K)$; poor correlation coefficient (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.30 (20°C, shake flask-UV, Korenman 1973)
 2.42 (23 ± 1.5°C, shake flask-LSC, Banerjee et al. 1980; Veith et al. 1980)

- 2.30 (shake flask, Korenman et al. 1980)
- 1.99, 2.54 (RP-HPLC-RT correlation, quoted calculated value, Veith et al. 1980)
- 2.54 (35°C, shake flask-UV, Rogers & Wong 1980)
- 2.34 (generator column-HPLC, Wasik et al. 1981)
- 2.37 (calculated-activity coeff. γ from UNIFAC not considering mutual solubility of octanol and water, Arbuckle 1983)
- 2.95 (calculated-activity coeff. γ from UNIFAC by considering mutual solubility of octanol and water, Arbuckle 1983)
- 2.14 (HPLC- k' correlation, Haky & Young 1984)
- 1.83 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
- 2.35 (recommended, Sangster 1989, 1993)
- 2.48 (calculated-UNIFAC activity coeff., Dallos et al. 1993)
- 2.30 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 1.18 (bluegill sunfish, Barrows et al. 1980)
- 2.18 (bluegill sunfish, Veith et al. 1980)
- 1.86 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.88 (calculated-MCI χ , Sabljic 1987a)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.98 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
- 2.63 (soil, calculated- K_{OW} , Lyman et al. 1982)
- 2.19 (activated carbon, Blum et al. 1994)
- 1.76 (calculated- K_{OW} , Kollig 1993)
- 2.62, 2.77 (average values for sediments, soils, Delle Site 2001)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k < 4 \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, $1.1 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)
 photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 radicals with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 8.0 \text{ h}$ in air, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; selected, Howard 1989)

$k_{OH} = 71.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 2 \text{ K}$ (Atkinson 1989)

photooxidation $t_{1/2} = 1.19\text{--}11.9 \text{ h}$, based on estimated rate constant for the reaction with OH radical in air (Howard et al. 1991)

$k_{OH}(\text{calc}) = 51.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1993)

$k_{OH}(\text{calc}) = 5.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{exptl}) = 1.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (SAR structure-activity relationship, Kwok & Atkinson 1995)

Hydrolysis:

Biodegradation: average rate of biodegradation $28.2 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982); first-order rate constant $k = 1.0 \text{ d}^{-1}$ corresponding to $t_{1/2} = 0.7 \text{ d}$ in adapted activated sludge under aerobic conditions (Mills et al. 1982);

$t_{1/2}(\text{aq. aerobic}) = 24\text{--}168 \text{ h}$, based on aqueous aerobic screening test data (Petrasek et al. 1983; Chambers et al. 1963; selected, Howard et al. 1991); $t_{1/2}(\text{aq. anaerobic}) = 96\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

average $k(\text{exptl.}) = 0.0578 \text{ h}^{-1}$ compared to group contribution method predicted $k = 0.0758 \text{ h}^{-1}$ (nonlinear) and $k = 0.0646 \text{ h}^{-1}$ (linear) (Tabak & Govind 1993).

Biotransformation: rate constant for bacterial transformation of 1×10^7 mL cell⁻¹ h⁻¹ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 8.0$ h, based on reaction with photochemically produced hydroxyl radical in air (GEMS 1986; quoted, Howard 1989); photooxidation $t_{1/2} = 1.19$ – 11.9 h, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 77$ – 3840 h in water, based on reported reaction rate constants for RO₂ radical with the phenol class (Mill & Mabey 1985; quoted, Howard et al. 1991).

Groundwater: $t_{1/2} = 48$ – 336 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24$ – 168 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 14.1.1.6.1

Reported aqueous solubilities and Henry's law constants of 2,4-dimethylphenol at various temperatures

Aqueous solubility		Henry's law constant			
Erichsen & Dobbert 1955		Ashworth et al. 1988		Dohnal & Fenclová 1995	
shake flask-optical method		EPICS-GC		vapor-liquid equilibrium	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ /mol)	t/°C	H/(Pa m ³ /mol)
160	17000	10	840	75.9	4.338
170	33000	15	683	88.7	7.491
180	54000	20	1023	98.5	11.46
190	77000	25	500		
200	114000	30	380		
210	188000				
212	234000	log H = A – B/(T/K)			
213	279000		H/(atm m ³ /mol)		
213.5	335000	A	–16.34		
25	6200	B	–3307		
	extrapolated				

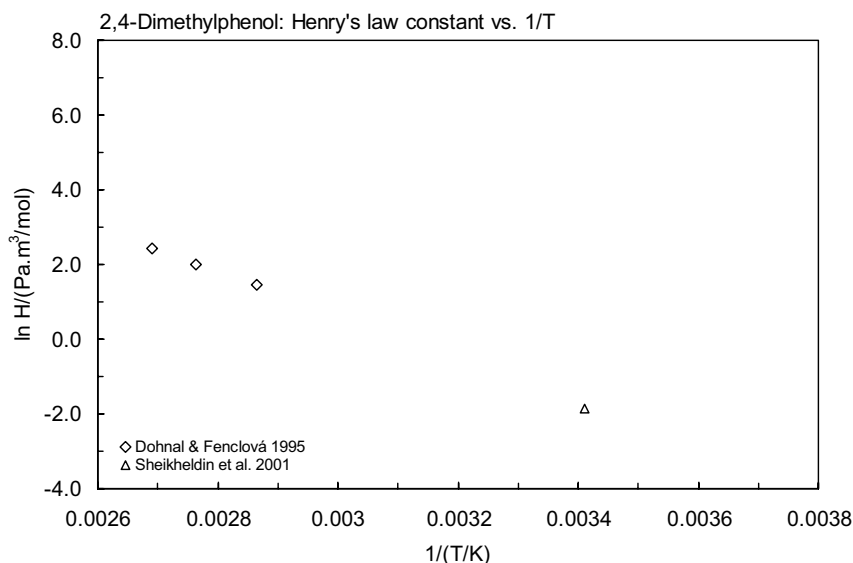


FIGURE 14.1.1.6.1 Logarithm of Henry's law constant versus reciprocal temperature for 2,4-dimethylphenol.

TABLE 14.1.1.6.2

Reported vapor pressures of 2,4-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/\text{K}) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Vonderres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.8	133.3	89.50	1333	9.73	3.040	144.382	13195
78.0	666.6	109.9	3333	14.94	5.066	156.053	20024
91.3	1333	127.0	6666	20.13	8.279	164.129	26289
105	2666	137.4	9999	24.87	12.81	171.241	33051
131.5	5333	144.5	13332	29.91	20.13	176.700	39155
131	7999	156.0	19998	35.16	30.797	182.116	46078
143	13332	165.1	26664	39.41	43.73	186.169	52557
161.5	26664	171.2	33330	44.86	67.06	191.348	60131
184.5	53329	177.3	39997			194.795	66188
211.5	101325	180.0	46663	mp/°C	24.54	198.444	73115
		186.7	53329	bp/°C	210.931	201.747	79877
mp/°C	25.5	190.8	59995			204.809	86584
		194.4	66661	for temp range:		207.513	92867
		198.0	73327	9–45°C		208.299	94764
		201.0	79993	eq. 2	P/mmHg	208.898	97557
		204.0	86659	A	10.5277	209.314	97251
		206.6	93325	B	3499.99	209.847	98580
		211.0	101325	C	273	210.45	100102
						210.951	101381

(Continued)

TABLE 14.1.1.6.2 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				$\Delta H_v/(\text{kJ mol}^{-1})$		211.453	102666
				at 25°C	65.856	211.888	103803
				at bp	47.145	212.32	106266
						for temp range:	
						144–212°C	
						eq. 2	P/mmHg
						A	7.04694
						B	1581.391
						C	168.652

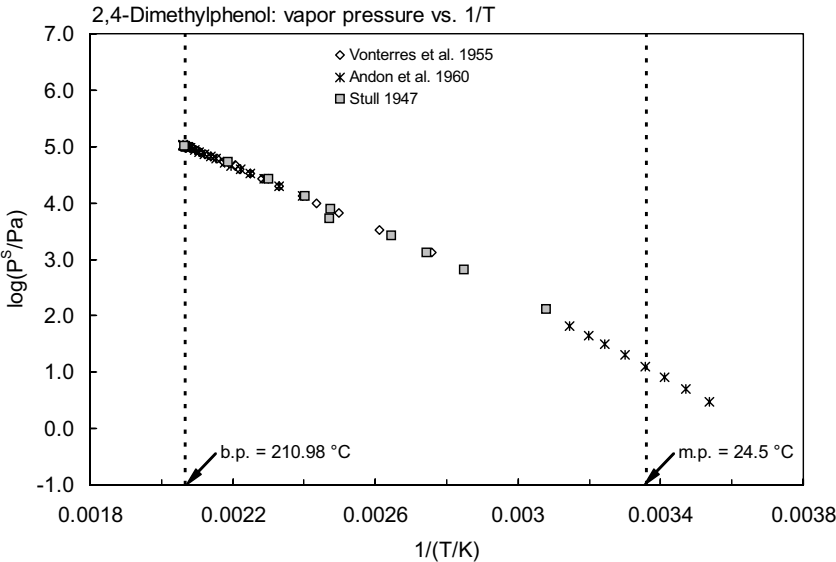
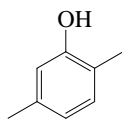


FIGURE 14.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dimethylphenol.

14.1.1.7 2,5-Dimethylphenol



Common Name: 2,5-Dimethylphenol

Synonym: 2,5-xylenol, 1-hydroxy-2,5-dimethylbenzene

Chemical Name: 2,5-dimethyl phenol

CAS Registry No: 95-87-4

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

74.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

211.1 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.41 (Dohnal & Fenclová 1995)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

84.98, 46.94 ($25^{\circ}C$, normal bp, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.325 (mp at $74.8^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

3126 (shake flask-UV, pH 5.1, Blackman et al. 1955)

3122 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($51.8^{\circ}C$, summary of literature data, temp range 51.8 – $211.5^{\circ}C$, Stull 1947)

1333* ($89.40^{\circ}C$, ebulliometry, measured range 89.40 – $211.2^{\circ}C$, Vonterres et al. 1955)

1.213* ($24.82^{\circ}C$, ebulliometry/gas saturation, measured range 9.5 – $45^{\circ}C$, Andon et al. 1960)

$\log(P/mmHg) = 13.3705 - 4438.56/(t/^{\circ}C + 273)$; temp range 9 – $50^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 7.03684 - 1581.906/(t/^{\circ}C + 169.497)$; temp range 143 – $212^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/kPa) = 6.1332 - 1560.465/(176.024 + t/^{\circ}C)$, temp range 144 – $211.2^{\circ}C$ (Antoine eq. derived from exptl data of Andon et al. 1960, Boublik et al. 1984)

$\log(P/kPa) = 6.04303 - 1383.881/(157.333 + t/^{\circ}C)$; temp range 89.4 – $211.2^{\circ}C$ (Antoine eq. derived from exptl data of Vonterres et al. 1955, Boublik et al. 1984)

$\log(P_s/kPa) = 12.51064 - 3950.681/(T/K)$, temp range 282 – $323 K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.17702 - 1593.804/(-102.241 + T/K)$; temp range 427 – $485 K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = 47.5888 - 4.8102 \times 10^3/(T/K) - 13.186 \cdot \log(T/K) - 1.0208 \times 10^{-9} \cdot (T/K) + 2.7045 \times 10^{-12} \cdot (T/K)^2$; temp range 348 – $707 K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant (Pa m³/mol at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0873, 0.133 (20, 25°C, calculated-limiting activity coefficient γ^∞ data, Dohnal & Fenclová 1995)

4.353, 7.476, 11.20 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

$\ln K_{AW} = 12.004 - 6511/(T/K)$; temp range 20–98.5°C (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.34 (shake flask, Korenman 1973)

2.33 (shake flask, Korenman et al. 1980)

2.35 (generator column-HPLC, Wasik et al. 1981)

2.34 (recommended, Sangster 1993)

2.48 (HPLC-RT correlation, Makovskaya et al. 1995b)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.1.7.1

Reported vapor pressures of 2,5-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)					
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Stull 1947		Vonderres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
51.8	133.3	89.40	1333	9.42	0.60	143.024	12990
78.0	666.6	109.8	3333	15.01	1.215	154.805	19234
91.3	1333	126.8	6666	19.9	2.186	164.433	26584
105	2666	137.2	9999	24.82	3.946	171.549	33375
121.5	5333	144.5	13333	29.83	6.849	176.902	39361
131	7999	156.0	19998	35.33	12.59	182.455	46460
143	13332	164.8	26666	39.41	19.47	187.328	53509
161.5	26664	171.5	33330	44.79	34.53	191.46	60142
184.2	53329	177.4	39997	49.75	52.80	194.984	66312
211.5	101325	180.2	43330			198.93	73602
		182.5	46663			210.834	79735
mp/°C	74.5	186.6	53329	mp/°C	74.85	204.603	85737
		189.5	59995	bp/°C	211.132	207.748	92988
		194.2	66661			208.661	95182
		198.0	73327	for temp range:		209.138	96349
		201.0	79993	9–50°C		209.556	97373

(Continued)

TABLE 14.1.1.7.1 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		204.6	86659	eq. 2	P/mmHg	210.117	98764
		206.8	93325	A	13.3705	210.771	100257
		211.2	101325	B	4438.56	211.232	101580
				C	273	211.736	102870
				ΔH_v /(kJ mol ⁻¹)		for temp range:	
				at 25°C	84.98	143–212°C	
				at bp	46.94	eq. 2	P/mmHg
						A	7.03684
						B	1581.906
						C	169.497

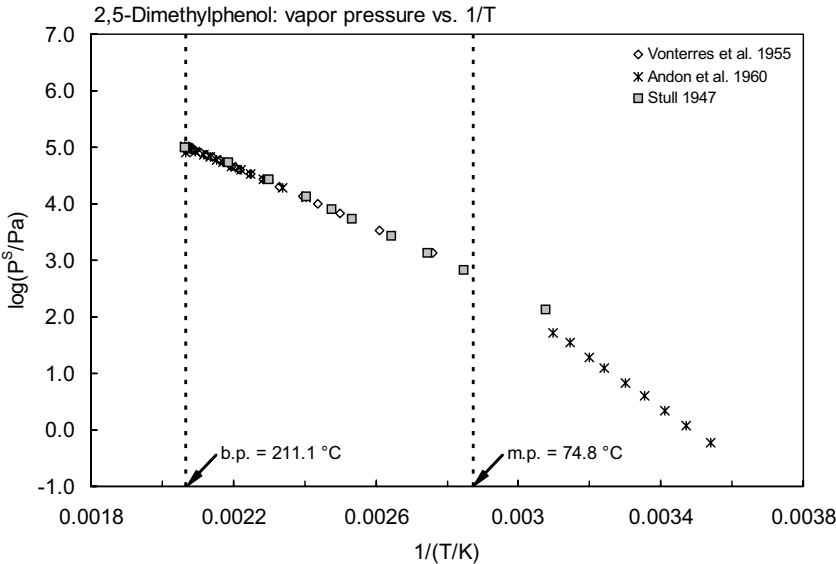
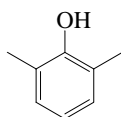


FIGURE 14.1.1.7.1 Logarithm of vapor pressure versus reciprocal temperature for 2,5-dimethylphenol.

14.1.1.8 2,6-Dimethylphenol



Common Name: 2,6-Dimethylphenol

Synonym: 2,6-xylenol, *vic-m*-xylenol

Chemical Name: 2,6-dimethylphenol

CAS Registry No: 576-26-1

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

45.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

201.07 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):1.1320 ($25^{\circ}C$, Andon et al. 1960)Molar Volume (cm^3/mol):107.9 ($25^{\circ}C$, calculated-density)

147.8 calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.60 (McLeese et al. 1979; Dean 1985; Varhaníčková et al. 1995)

10.63 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):60.41, 46.97 ($25^{\circ}C$, bp, Dreisbach 1955)

44.52 (at normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):75.6 (at $25^{\circ}C$, Andon et al. 1960; Dean 1992)Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.9; 16.3 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$.), F: 0.625 (mp at $45.8^{\circ}C$)Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6230 (shake flask-UV at pH 5.1, Blackman et al. 1955)

13000* ($130^{\circ}C$, shake flask-optical method, measured range 130 – $241.2^{\circ}C$, Erichsen & Dobbert 1955)

9650 (generator column-HPLC, Wasik et al. 1981)

2900, 5900 (8, $25^{\circ}C$, Leuenberger et al. 1985)9560 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

6150 (shake flask-HPLC/UV at pH 6.3, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

19.086 (calculated-Antoine eq., Dreisbach 1955)

 $\log(P/mmHg) = 7.40318 - 1858.7/(199.0 + t/^{\circ}C)$; temp range 115 – $250^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)1333* ($92.5^{\circ}C$, ebulliometry, measured range 92.5 – $212.0^{\circ}C$, Vonterres et al. 1955)23.3* ($24.67^{\circ}C$, ebulliometric and gas-saturation methods, measured range 4.75 – $40^{\circ}C$, Andon et al. 1960)

24.31 (calculated-Antoine eq. from ebulliometry/gas saturation measurements, Andon et al. 1960)

 $\log(P/mmHg) = 12.5036 - 3948.27/(t/^{\circ}C + 273)$; temp range 4 – $40^{\circ}C$ (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960) $\log(P/mmHg) = 7.05753 - 1618.528/(t/^{\circ}C + 186.482)$; temp range 144 – $203^{\circ}C$ (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)

- 34.41 (extrapolated-Antoine eq., Boublik et al. 1973)
 $\log (P/\text{mmHg}) = 7.0707 - 1628.323/(187.603 + t/^{\circ}\text{C})$, temp range 144.8–203.5°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
- 33.68 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 474.112/(T/K)] \times 10^{\{0.99333 - 9.96552 \times 10^{-4} \cdot (T/K) + 8.34247 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 321.81–701.65 K (Cox eq., Chao et al. 1983)
- 34.41, 10.37 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.19572 - 1628.413/(187.613 + t/^{\circ}\text{C})$, temp range 144.8–203.5°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.57979 - 1831.266/(188.83 + t/^{\circ}\text{C})$, temp range 97.5–212°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 34.4 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 7.00707 - 1628.32/(187.60 + t/^{\circ}\text{C})$; temp range 145–204°C (Antoine eq., Dean 1985, 1992)
- 19.09 (selected, Riddick et al. 1986)
- 24.0 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.6308 - 3950.681/(T/K)$; temp range 277–313 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.19544 - 1629.621/(-85.358 + T/K)$; temp range 417–476 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
- 43.8 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 39.83138 - 4062.725/(T/K) - 10.16994 \cdot \log (T/K) + 0.20170 \times 10^{-2} \cdot (T/K)$; temp range: 418–477 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1960, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 87.1964 - 5.8721 \times 10^3/(T/K) - 28.853 \cdot \log (T/K) + 1.113 \times 10^{-2} \cdot (T/K) + 2.2316 \times 10^{-12} \cdot (T/K)^2$; temp range 319–701 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 0.684 (modified gas-stripping, Hawthorne et al. 1985)
 0.193 (8°C, Leuenberger et al. 1985)
 0.377 (calculated-P/C, Shiu et al. 1994)
 0.302 (calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)
 10.3, 17.81, 25.2 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
 0.441 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
 $\ln K_{AW} = 11.176 - 5906/(T/K)$, temp range 20–100°C (vapor-liquid equilibrium measurements with additional lit. data, Dohnal & Fenclová 1995)
 0.098 (calculated-group contribution, Lee et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$ at 25°C or as indicated:

- 2.36 (Leo et al. 1971; Hansch & Leo 1979)
 2.34 (LC- k' correlation; Carlson et al. 1975)
 2.40 (35°C, shake flask-UV, Rogers & Wong 1980)
 2.31 (generator column-HPLC, Wasik et al. 1981)
 2.07 (HPLC- k' correlation, Haky & Young 1984)
 2.51 (HPLC-RT correlation, Eadsforth 1986)
 2.36 (recommended, Sangster 1989, 1993)
 2.36 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 65.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 54.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Atmospheric Oxidation Program, $k_{OH}(\text{exptl}) = 65.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; and $k_{OH}(\text{calc}) = 30.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ estimated from Fate of Atmospheric Pollutants Program (Meylan & Howard 1993)

$k_{OH}(\text{calc}) = 49.48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

Hydrolysis:

Biodegradation: $t_{1/2} = 7\text{--}10 \text{ d}$ for bacteria to utilize 95% of 200 ppm in parent substrate (Tabak et al. 1964); average rate of biodegradation $9.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 14.1.1.8.1

Reported aqueous solubilities and vapor pressures of 2,6-dimethylphenol at various temperatures

$\log P = A - B/(T/K)$		(1)		$\ln P = A - B/(T/K)$		(1a)	
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)		$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)	
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)					
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Aqueous solubility		Vapor pressure					
Erichsen & Dobbert 1955		Vonterres et al. 1955		Andon et al. 1960			
shake flask-optical method		ebulliometry		gas saturation		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
130	13000	92.5	1333	4.75	2.60	144.798	19813
140	16000	112.5	3333	9.46	4.48	153.385	26322
150	21000	129.0	6666	14.98	8.319	160.524	33079
160	27000	139.4	9999	19.78	13.87	166.759	39853
170	36000	147.1	13332	24.67	23.33	171.831	46274
180	47000	158.4	19998	30.2	39.86	176.276	52564
190	58000	167.0	26664	34.98	64.93	180.369	59847
200	71000	173.2	33330	39.66	100.3	184.792	66529
210	90000	179.1	39997			188.694	73851
220	120000	181.5	43330	mp/°C	74.85	191.754	80043
230	176000	188.0	53329	bp/°C	201.03	194.81	86616
232	191000	190.2	59995			196.676	90843
234	209000	196.3	66661	for temp range:		198.414	94918
236	229000	200.0	73327	4–40°C		198.937	96176
238	255000	202.5	79993	eq. 2	P/mmHg	199.432	97373
240	297000	205.6	86659	A	12.5036	199.983	98721
241.2	440000	208.0	93325	B	3948.27	200.45	99881
		212.0	101325	C	273	201.059	101400
						201.616	120808
				$\Delta H_V/(\text{kJ mol}^{-1})$		202.519	105117
				at 25°C	75.60	203.525	107738
				at bp	44.52		

TABLE 14.1.1.8.1 (Continued)

Aqueous solubility		Vapor pressure					
Erichsen & Dobbert 1955		Vonterres et al. 1955		Andon et al. 1960			
shake flask-optical method		ebulliometry		gas saturation		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
for temp range: 144–203°C							
eq. 2						P/mmHg	
A						7.05753	
B						1618.528	
C						186.492	

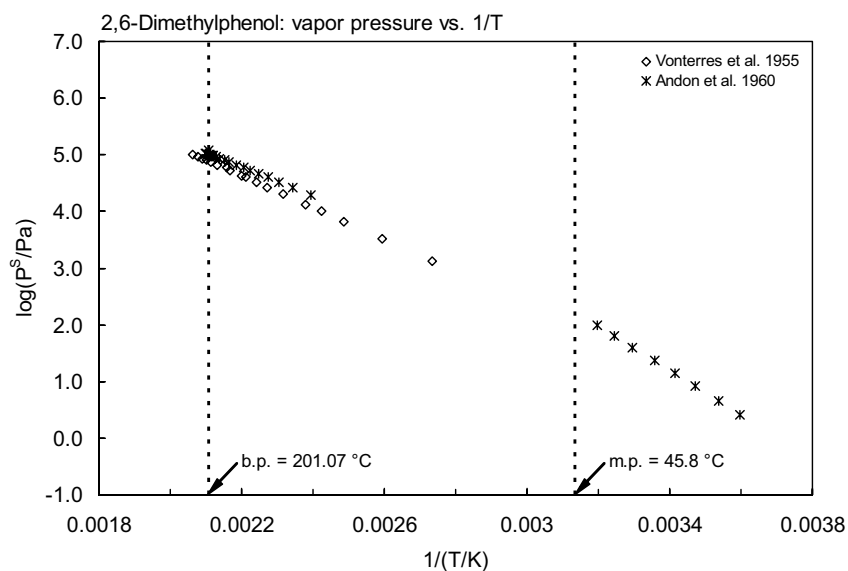
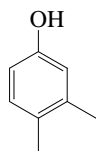


FIGURE 14.1.1.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dimethylphenol.

14.1.1.9 3,4-Dimethylphenol



Common Name: 3,4-Dimethylphenol

Synonym: 3,4-xylenol, *as-o*-xylenol

Chemical Name: 3,4-dimethylphenol

CAS Registry No: 95-65-8

Molecular Formula: $C_8H_{10}O$, $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

65.1 (Lide 2003)

Boiling Point ($^{\circ}C$):

227 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1380 ($25^{\circ}C$, Andon et al. 1960)

0.9830 (Weast 1982–83)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.40 (McLeese et al. 1979)

10.32 (Dean 1985)

10.36 (Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

49.67 (at normal boiling point, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

85.73 (at $25^{\circ}C$, Andon et al. 1960; Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.13; 17.0 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.404 (mp at $65.1^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5100 (shake flask-UV, Blackman et al. 1955)

5100* (synthetic method/shake flask-optical, extrapolated value, measured range 130 – $190.2^{\circ}C$, Ericksen & Dobbert 1955)

5000 (shake flask-spectrophotometry, Roberts et al. 1977)

12810 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

7250 (shake flask-HPLC/UV at pH 6.25, Varhaničková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($66.2^{\circ}C$, summary of literature data, temp range 66.2 – $225.2^{\circ}C$, Stull 1946)

5.160 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.70494 - 2030.9/(196.0 + t/^{\circ}C)$; temp range 130 – $265^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

- 1333* (105.7 °C, ebulliometry, measured range 105.7–226.0°C, Vonterres et al. 1955)
- 1.84* (24.88°C, ebulliometry/gas-saturation methods, measured range 9.89–49.36°C, Andon et al. 1960)
- 1.895 (interpolated-Antoine eq. from ebulliometry/gas saturation measurements, Andon et al. 1960)
- $\log (P/\text{mmHg}) = 13.1729 - 4478.23/(t/^{\circ}\text{C} + 273)$; temp range: 9–50°C, (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)
- $\log (P/\text{mmHg}) = 7.07343 - 1617.202/(t/^{\circ}\text{C} + 158.778)$; temp range 171–229°C (Antoine eq., ebulliometric and gas-saturation measurements, Andon et al. 1960)
- $\log (P/\text{mmHg}) = [-0.2185 \times 13991.0/(T/\text{K})] + 9.02680$; temp range 66.2–225.2°C (Antoine eq., Weast 1972–73)
- 2.541 (extrapolated-Antoine eq., Boublik et al. 1973)
- $\log (P/\text{mmHg}) = 7.07979 - 1621.451/(159.261 + t/^{\circ}\text{C})$; temp range 172–228°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1973)
- 3.621 (extrapolated-Cox eq., Chao et al. 1983)
- $\log (P/\text{mmHg}) = [1 - 499.926/(T/\text{K})] \times 10^{1.05062 - 10.2129 \times 10^{-4} \cdot (T/\text{K}) + 8.04338 \times 10^{-7} \cdot (T/\text{K})^2}$; temp range: 353.20–729.65 K, (Cox eq., Chao et al. 1983)
- 7.327 (supercooled liquid P_L , extrapolated-Antoine eq., Boublik et al. 1984)
- $\log (P/\text{kPa}) = 6.20545 - 1622.411/(159.947 + t/^{\circ}\text{C})$; temp range 172–228°C (Antoine eq. from reported exptl. data of Andon et al. 1960, Boublik et al. 1984)
- $\log (P/\text{kPa}) = 7.46831 - 2538.736/(239.359 + t/^{\circ}\text{C})$; temp range 105.7–226°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
- 2.540 (extrapolated-Antoine eq., Dean 1985)
- $\log (P/\text{mmHg}) = 7.07919 - 1621.45/(159.26 + t/^{\circ}\text{C})$; temp range 172–229°C (Antoine eq., Dean 1985, 1992)
- 5.160 (Riddick et al. 1986)
- 1.865 (solid P_S , interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log (P_S/\text{kPa}) = 12.31521 - 4485.592/(T/\text{K})$; temp range 282–323 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
- $\log (P_L/\text{kPa}) = 6.20617 - 1623.592/(-113.623 + T/\text{K})$; temp range 444–502 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
- 3.795 (extrapolated-four parameter vapor pressure eq., Nesterova et al. 1990)
- $\log (P/\text{Pa}) = 93.28460 - 6735.317/(T/\text{K}) - 29.48566 \cdot \log (T/\text{K}) + 0.95432 \times 10^{-2} \cdot (T/\text{K})$; temp range: 445–502 K (four-parameter vapor pressure eq. derived using exptl data of Andon et al. 1950, Nesterova et al. 1990)
- $\log (P/\text{mmHg}) = 68.6521 - 6.15 \times 10^3/(T/\text{K}) - 20.184 \cdot \log (T/\text{K}) - 1.1259 \times 10^{-10} \cdot (T/\text{K}) + 4.0266 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 338–730 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 0.00942 (Leuenberger et al. 1985)
- 0.0212 (calculated-P/C, Shiu et al. 1994)
- 0.0278 (20°C, calculated-activity coeff. γ^{∞} data, Dohnal & Fenclová 1995)
- 1.416, 2.903, 4.619 (75.9, 88.7, 98.5°C, vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)
- 0.0421 (extrapolated-vapor-liquid equilibrium measurements, Dohnal & Fenclová 1995)
- $\ln K_{AW} = 11.854 - 6809/(T/\text{K})$, temp range 20–100°C (vapor-liquid equilibrium VLE measurements with additional lit. data, Dohnal & Fenclová 1995)
- 0.098 (calculated-group contribution, Lee et al. 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.23 (20°C, shake flask-UV, Korenman 1973)
- 2.23 (shake flask, Korenman et al. 1980)
- 2.23 (recommended, Sangster 1989, 1993)
- 2.23 (recommended, Hansch et al. 1995)
- 2.36 (HPLC-RT correlation, Makovskaya et al. 1995b)
- 2.26 (solid-phase micro-extraction, Dean et al. 1996)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{OH} = 81.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1989)

$k_{OH}(\text{calc}) = 55.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

Biodegradation: average rate of biodegradation $13.4 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 14.1.1.9.1

Reported aqueous solubilities of 3,4-dimethylphenol at various temperatures

Erichsen & Dobbert 1955

shake flask-optical method	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
130	29000
140	36000
150	42000
160	59000
170	81000
180	124000
186	173000
188	200000
189	222000
190	278000
190.2	336000
25	5100*
*extrapolated	

TABLE 14.1.1.9.2

Reported vapor pressures of 3,4-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1)$$

$$\ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^\circ\text{C}) \quad (2)$$

$$\ln P = A - B/(C + t/^\circ\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947

Vonterres et al. 1955

Andon et al. 1960

summary of literature data		ebulliometry		gas saturation		ebulliometry	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
66.2	133.3	105.7	1333	9.89	0.293	171.933	20341
93.8	666.6	125.8	3333	14.78	0.543	180.131	26703
107.7	1333	142.6	6666	19.98	1.031	186.548	32749

(Continued)

TABLE 14.1.1.9.2 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
122	2666	152.9	9999	24.88	1.840	193.38	40369
138	5333	160.9	13332	29.8	3.240	197.879	46135
148	7999	172.3	19998	34.86	5.626	202.37	52526
162	13332	180.3	26664	39.67	9.386	207.376	60478
181.5	26664	187.7	33330	44.76	16.13	211.126	67049
203.6	53329	193.9	39997	49.36	25.46	213.126	72703
225.2	101325	196.3	43330			217.587	79685
		198.7	46663	mp/°C	65.11	200.898	86882
mp/°C	62.8	203.0	53339	bp/°C	221.692	223.649	93227
		212.5	66661			224.292	94764
		213.4	73327	for temp range:		224.799	95996
		216.5	79993	9–50°C		225.276	97153
		219.2	86659	eq. 2	P/mmHg	225.928	98771
		222.0	93325	A	13.1729	226.392	99920
		226.0	101325	B	4478.23	226.921	101242
				C	273	227.397	102474
						228.487	105289
				ΔH_v /(kJ mol ⁻¹)		228.899	106371
				at 25°C	85.73		
				at bp	49.67	for temp range:	
						171–229°C	
						eq. 2	P/mmHg
						A	7.07343
						B	1617.202
						C	158.778

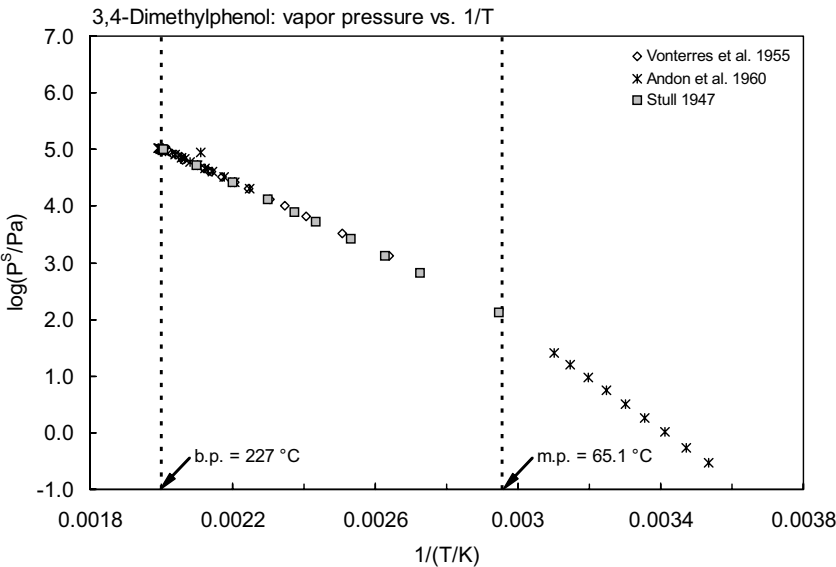
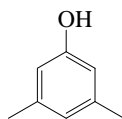


FIGURE 14.1.1.9.1 Logarithm of vapor pressure versus reciprocal temperature for 3,4-dimethylphenol.

14.1.1.10 3,5-Dimethylphenol



Common Name: 3,5-Dimethylphenol

Synonym: 3,5-xylenol, 1-hydroxy-3,5-dimethylbenzene

Chemical Name: 3,5-dimethyl phenol

CAS Registry No: 108-68-9

Molecular Formula: $C_8H_{10}O$ $CH_3C_6H_3(CH_3)OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

63.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

221.74 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constants, pK_a :

7.8 (McLeese et al. 1979)

10.19 (Dohnal & Fenclová 1995)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

82.84, 49.31 ($25^{\circ}C$, normal bp, Andon et al. 1960)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.420$ (mp at $63.4^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

4886 (shake flask-UV, pH 5.1, Blackman et al. 1955)

4425 ($20^{\circ}C$, shake flask-UV, Dohnal & Fenclová 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($62.0^{\circ}C$, summary of literature data, temp range 62 – $219.5^{\circ}C$, Stull 1947)

1333* ($102.8^{\circ}C$, ebulliometry, measured range 102.8 – $219.0^{\circ}C$, Vonterres et al. 1955)

2.63* ($24.95^{\circ}C$, ebulliometry/gas saturation, measured range 9 – $45^{\circ}C$, Andon et al. 1960)

$\log(P/mmHg) = 12.8271 - 4328.13/(t/^{\circ}C + 273)$; temp range 9 – $50^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/mmHg) = 7.11745 - 1630.124/(t/^{\circ}C + 163.076)$; temp range 154 – $224^{\circ}C$ (Antoine eq. from ebulliometric and gas-saturation measurements, Andon et al. 1960)

$\log(P/kPa) = 6.25752 - 1641.206/(164.311 + t/^{\circ}C)$, temp range 154.7 – $223.3^{\circ}C$ (Antoine eq. derived from reported exptl data of Andon et al. 1960, Boublik et al. 1984)

$\log(P/kPa) = 8.27972 - 3182.232/(287.862 + t/^{\circ}C)$, temp range 102.8 – $219^{\circ}C$ (Antoine eq. derived from reported exptl data of Vonterres et al. 1960, Boublik et al. 1984)

$\log(P_s/kPa) = 11.97153 - 4336.025/(T/K)$; temp range 282 – $323\ K$ (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.25292 - 1638.564/(-109.095 + T/K)$; temp range 427 – $497\ K$ (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -44.915 - 2.8912 \times 10^3/(T/K) + 25.704 \cdot \log(T/K) - 3.9714 \times 10^{-2} \cdot (T/K) + 1.6464 \times 10^{-5} \cdot (T/K)^2$; temp range 337 – $716\ K$ (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

0.0419, 0.0614 (20, 25°C , calculated-limiting activity coefficient γ^∞ data, Dohnal & Fenclová 1995)

1.95, 3.70, 6.12 (75.9, 88.7, 98.5°C , vapor-liquid equilibrium-GC, Dohnal & Fenclová 1995)

$\ln K_{\text{AW}} = 11.654 - 6636/(T/\text{K})$; temp range $20\text{--}98.5^\circ\text{C}$ (vapor-liquid equilibrium VLE data, Dohnal & Fenclová 1995)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.31 (shake flask, Korenman 1972; Korenman et al. 1980)

2.55 (shake flask-UV, Rogers & Wong 1980)

2.38 (UNIFAC activity coefficient, Campbell & Luthy 1985)

2.54 (HPLC-RT correlation, Eadsforth 1986)

2.35 (shake flask, Log P Database, Hansch & Leo 1987)

2.35 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$ or $\log K_{\text{B}}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

Half-Lives in the Environment:

TABLE 14.1.1.10.1

Reported vapor pressures of 3,5-dimethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log (P/\text{Pa}) = A - B/(C + T/K)$	(3)						
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Stull 1947	Vonnerres et al. 1955	Andon et al. 1960					
summary of literature data	ebulliometry	gas saturation	ebulliometry				
t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa	t/^{\circ}C	P/Pa
62	133.3	102.8	1333	9.57	0.44	154.72	12984
89.2	666.6	122.5	3333	14.92	0.813	166.472	19760
102.4	1333	139.1	6666	20.35	1.587	175.126	26444
117.0	2666	149.0	9999	24.05	2.626	182.389	33392
133.3	5333	156.8	13332	30.42	4.866	187.937	39757
143.5	7999	168.1	19998	34.85	7.813	192.743	45815
156	13332	176.3	26664	39.94	13.32	197.298	52352
176.2	26664	182.9	33330	45.23	22.80	201.925	59794
197.8	53329	188.5	39997	49.97	35.33	205.601	66193
219.5	101325	191.0	43330			209.151	72942
		194.0	46663			212.159	79072
mp/^{\circ}C	68.0	198.1	53329	mp/^{\circ}C	63.27	215.799	87070
		202.0	59995	bp/^{\circ}C	221.692	218.298	92904
		205.3	66661			219.146	94952
		208.3	73327	for temp range:		219.584	96027
		211.0	79993	9–50^{\circ}C		220.097	97296
		214.0	86659	eq. 2	P/mmHg	220.692	98771

TABLE 14.1.1.10.1 (Continued)

Stull 1947		Vonterres et al. 1955		Andon et al. 1960			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		216.2	93325	A	12.8271	221.309	100334
		219.0	101325	B	4328.13	221.709	101362
				C	273	222.269	102845
						222.724	104007
						223.321	105573
				ΔH_v /(kJ mol ⁻¹)			
				at 25°C			
				82.84			
				at bp			
				49.31		for temp range:	
						154–224°C	
						eq. 2	P/mmHg
						A	7.11745
						B	1630.124
						C	163.076

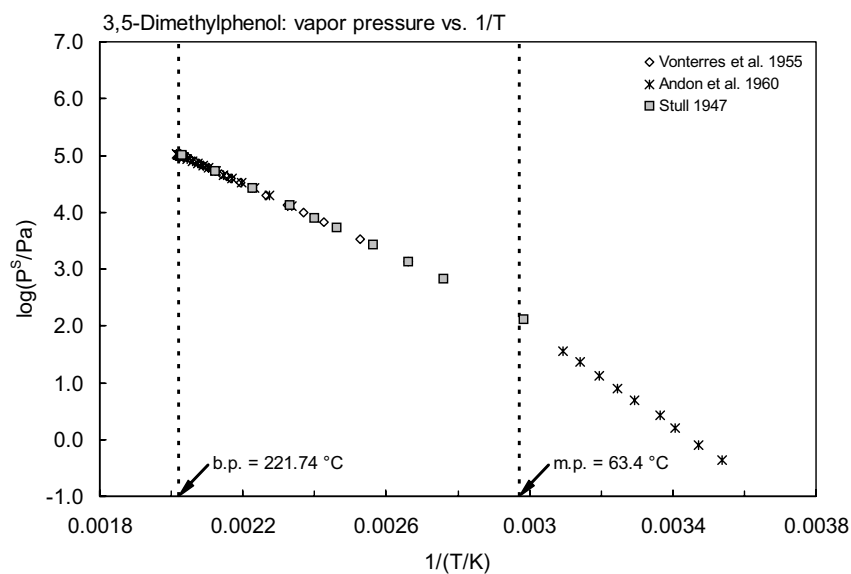
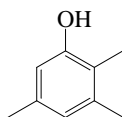


FIGURE 14.1.1.10.1 Logarithm of vapor pressure versus reciprocal temperature for 3,5-dimethylphenol.

14.1.1.11 2,3,5-Trimethylphenol



Common Name: 2,3,5-Trimethylphenol

Synonym:

Chemical Name: 2,3,5-trimethylphenol

CAS Registry No: 697-82-5

Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

94.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

233 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.60 (Blackman et al. 1955)

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.208 (mp at $94.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

40000* (200 $^{\circ}C$, synthetic method/shake flask-optical, measured range 200–248 $^{\circ}C$, Erichsen & Dobbert 1955)

762 (shake flask-UV, Blackman et al. 1955)

855 (shake flask-HPLC/UV at pH 5.95, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

2.426* (extrapolated-Antoine eq., ebulliometry, measured range 186–247 $^{\circ}C$, Handley et al. 1964)

$\log (P/mmHg) = 7.08022 - 1685.973/(166.150 + t/^{\circ}C)$; temp range 186–247 $^{\circ}C$ (Antoine eq., ebulliometric method, Handley et al. 1964)

4.451 (extrapolated-Cox eq., Chao et al. 1983)

$\log (P/mmHg) = [1 - 508.477/(T/K)] \times 10^{0.932965 - 5.75276 \times 10^{-4} \cdot (T/K) + 3.29737 \times 10^{-7} \cdot (T/K)^2}$; temp range: 459.63–520.21 K, (Cox eq., Chao et al. 1983)

2.426 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log (P/mmHg) = 7.08012 - 1685.896/(166.141 + t/^{\circ}C)$, temp range 186.5–247 $^{\circ}C$ (Antoine eq. from reported exptl. data of Handley et al. 1964, Boublik et al. 1984)

2.43, 0.0234 (extrapolated from liquid, Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.02493 - 1685.528/(166.133 + t/^{\circ}C)$, temp range 186.5–247 $^{\circ}C$ (Antoine eq. from reported exptl. data of Handley et al. 1964, Boublik et al. 1984)

$\log (P/kPa) = 6.95436 - 889.02/(67.752 + t/^{\circ}C)$, temp range 106–233 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

2.43 extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 7.08012 - 1685.90/(166.14 + t/^{\circ}C)$, temp range 186–247 $^{\circ}C$ (Antoine eq., Dean 1985, 1992)

2.44 (extrapolated, liquid, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.20676 - 1687.869/(-106.761 + T/K)$, temp range 459–531 K (Antoine eq., Stephenson & Malanowski 1987)

$\log (P/\text{Pa}) = 89.62984 - 6541.396/(T/\text{K}) - 28.26318 \cdot \log (T/\text{K}) + 0.92991 \times 10^{-2} \cdot (T/\text{K})$; temp range: 460–520 K
(four-parameter vapor pressure eq. derived using exptl data of Handley et al. 1964, Nesterova et al. 1990)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.404 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.06 (COMPUTOX databank, Kaiser 1993)

2.92 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.61 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

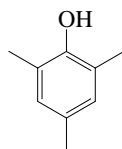
TABLE 14.1.1.11.1
Reported aqueous solubilities and vapor pressures of 2,3,5-trimethylphenol at various temperatures

Aqueous solubility		Vapor pressure	
Erichsen & Dobbert 1955		Handley et al. 1964	
shake flask-optical method		ebulliometry	
$t/^{\circ}\text{C}$	$S/\text{g} \cdot \text{m}^{-3}$	$t/^{\circ}\text{C}$	P/Pa
200	40000	186.482	26547
210	54000	193.614	33021
220	79000	200.127	40002
230	128000	205.448	46560
240	200000	210.422	53453
242	224000	214.675	59972
244	250000	218.644	66623
246	291000	222.382	73417
257.8	420000	225.707	79909
		229.041	86877
		231.852	93116
		234.759	99940
		237.50	106735
		240.13	113587
		242.511	120090
		244.811	126646
		247.062	133344
		mp/ $^{\circ}\text{C}$	93.73
		bp/ $^{\circ}\text{C}$	235.329

TABLE 14.1.1.11.1 (Continued)

Aqueous solubility		Vapor pressure	
Erichsen & Dobbert 1955		Handley et al. 1964	
shake flask-optical method		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	P/Pa
for temp range: 186–247°C			
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$			
			P/mmHg
A			7.08022
B			1685.973
C			166.150
$\Delta H_v/(\text{kJ mol}^{-1})$			
at bp			49.96

14.1.1.12 2,4,6-Trimethylphenol



Common Name: 2,4,6-Trimethylphenol

Synonym: Mesityl

Chemical Name: 2,4,6-Trimethylphenol

CAS Registry No: 527-60-6

Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

73 (Lide 2003)

Boiling Point ($^{\circ}C$):

220 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.90 (Blackman et al. 1955)

10.88 (Dean 1985)

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, $F: 0.338$ (mp at $73^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1007 (shake flask-UV, Blackman et al. 1955; quoted, Varhaničková et al. 1995)

1420 (shake flask-HPLC/UV at pH 4.85, Varhaničková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

7.0 (extrapolated from liquid state, Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.91352 - 1481.329/(158.589 + t/^{\circ}C)$, temp range $94-220.6^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

19.6 (supercooled liquid P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.82395 - 2158.2/(-45.2 + T/K)$, temp range $367-494 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.2512 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.73 (generator column-HPLC/UV, Wasik et al. 1981)

2.73 (quoted and recommended, Sangster 1989; 1993)

2.7 3 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

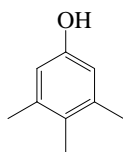
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.1.13 3,4,5-Trimethylphenol



Common Name: 3,4,5-Trimethylphenol

Synonym:

Chemical Name: 3,4,5-trimethylphenol

CAS Registry No: 527-54-8

Molecular Formula: $C_9H_{12}O$, $C_6H_2(CH_3)_3OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

108 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

249 (Stephenson & Malanowski 1987)

248.5 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

10.25 (Dean 1985)

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.153 (mp at $108^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1538 (shake flask-HPLC/UV, Varhaníčková et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P_L/kPa) = 7.33216 - 2536.1/(-44.56 + T/K)$, temp range 396–521 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

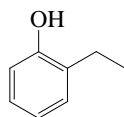
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.1.14 *o*-Ethylphenol

Common Name: 2-Ethylphenol

Synonym: *o*-ethylphenol

Chemical Name: 2-ethylphenol, *o*-ethylphenol

CAS Registry No: 90-00-6

Molecular Formula: C₈H₁₀O, C₂H₅C₆H₄OH

Molecular Weight: 122.164

Melting Point (°C):

18 (Lide 2003)

Boiling Point (°C): 204.52

204.5 (Lide 2003)

Density (g/cm³ at 20°C):

1.01885, 1.01459 (20°C, 25°C Biddiscombe et al. 1963)

1.0370 (Verschuereen 1983; 25°C, Dean 1985)

Molar Volume (cm³/mol):

117.8 (0°C, Stephenson & Malanowski 1987)

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a:

10.02 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

14040 (shake flask-HPLC/UV at pH 5.2, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (46.2 °C, summary of literature data, temp range 46.2–207.5°C, Stull 1947)

33.66 (calculated-Antoine eq., Dreisbach 1955)

log (P/mmHg) = 7.23343 – 1771.5/(200.0 + t/°C), temp range 105–245°C (Antoine eq. for liquid state, Dreisbach 1955)

20.84 (interpolated-Antoine eq., Biddiscombe et al. 1963)

20.4* (24.93°C, ebulliometric and gas transpiration measurements, measured range 5–45°C, Biddiscombe & Martin 1958)

log (P/mmHg) = 10.3131 – 3313.50/(t/°C + 273); temp range 5–45°C (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

log (P/mmHg) = 7.00742 – 1648.923/(t/°C + 170.833); temp range 150–218°C (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

log (P/mmHg) = [–0.2185 × 12516.7/(T/K)] + 8.586948; temp range 46.2–207.5°C (Antoine eq., Weast 1972–73)

log (P/mmHg) = [1– 480.731/(T/K)] × 10⁴{0.883881 – 6.07675 × 10^{–4}·(T/K) + 6.44264 × 10^{–7}·(T/K)²}; temp range: 319.35–480.65 K, (Cox eq., Chao et al. 1983)

16.7, 29 (extrapolated-Antoine eq., Boublik et al. 1984)

log (P/kPa) = 6.13214 – 1548.802/(170.82 + t/°C), temp range 150.4–215.05°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublik et al. 1984)

log (P/kPa) = 6.97225 – 2178.815/(231.035 + t/°C), temp range 86–207.5°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

27.01 (extrapolated-Antoine eq., Dean 1985)

log (P/mmHg) = 7.8003 – 2140.4/(227 + t/°C), temp range 86–208°C (Antoine eq., Dean 1985, 1992)

20.87 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.13344 - 1550.409/(-102.103 + T/\text{K})$; temp range 423–491 K (Antoine eq.-I, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 9.44878 - 3318.181/(T/\text{K})$, temp range 277–318 K (Antoine eq.-II, Stephenson & Malanowski 1987)

19.55 (extrapolated-Antoine eq., Nesterova et al. 1990)

$\log (P/\text{Pa}) = 94.95377 - 6350.841/(T/\text{K}) - 30.56287 \cdot \log (T/\text{K}) + 1.09475 \times 10^{-2} \cdot (T/\text{K})$; temp range: 424–491 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.174 (calculated with selected-P/C)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.47 (shake flask, Hansch & Leo 1979)

2.64 (shake flask, Korenman 1980)

2.64 (HPLC-RT correlation, Butte et al. 1981)

2.47 (recommended, Sangster 1989, 1993)

2.46 (HPLC-RT correlation, Ritter et al. 1994)

2.47 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.1.14.1

Reported vapor pressures of *o*-ethylphenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)		
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)		
$\log (P/\text{Pa}) = A - B/(C + T/K)$	(3)				
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$	(4)				
Stull 1947		Biddiscombe et al. 1963			
summary of literature data		gas saturation		ebulliometry	
t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa	t/^{\circ}\text{C}	P/Pa
46.2	133.3	4.98	3.346	150.425	20458
73.4	666.6	10.0	5.173	158.137	26542
87	1333	15.01	8.759	164.876	32996
101.5	2666	20.01	13.73	171.143	40086
117.9	5333	24.93	20.40	176.174	46627
127.9	7999	29.53	30.80	180.808	53390
141.8	13332	34.84	45.86	184.869	59946
161.6	26664	39.99	73.99	188.565	66460
184.5	53329	45.0	102.9	192.115	73235
207.5	101325			195.266	79702
				198.382	86528
mp/^{\circ}\text{C}	−45	mp/^{\circ}\text{C}	−3.31	200.845	92242

(Continued)

bp/°C		217.985	204.350	100866
TABLE 14.1.1.14.1 (Continued)				
Stull 1947		Biddiscombe et al. 1963		
summary of literature data		gas saturation		ebulliometry
t/°C	P/Pa	t/°C	P/Pa	t/°C P/Pa
				206.632 106865
		for temp range:		208.429 111753
		5–45°C		209.854 115762
		eq. 2	P/mmHg	212.651 123942
		A	10.3131	215.149 131641
		B	3313.50	218.047 142363
		C	273	
		ΔH _v /(kJ mol ⁻¹)		for temp range:
		at 25°C	63.60	150–218°C
		at bp	48.116	eq. 2 P/mmHg
				A 7.00742
				B 1548.923
				C 170.833

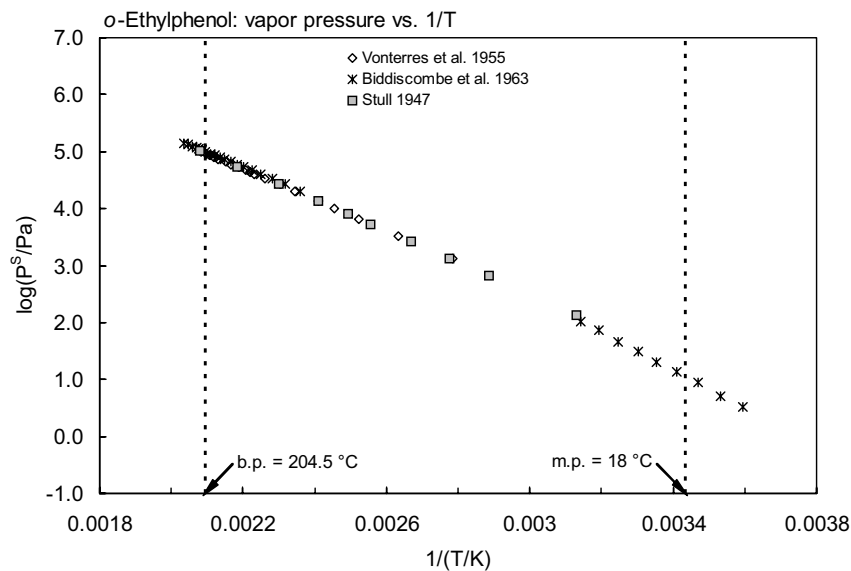
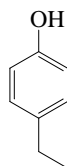


FIGURE 14.1.1.14.1 Logarithm of vapor pressure versus reciprocal temperature for o-ethylphenol.

14.1.1.15 *p*-Ethylphenol

Common Name: 4-Ethylphenol

Synonym: *p*-ethylphenol

Chemical Name: 2-ethylphenol, *p*-ethylphenol

CAS Registry No: 123-07-9

Molecular Formula: $C_8H_{10}O$, $C_2H_5C_6H_4OH$

Molecular Weight: 122.164

Melting Point ($^{\circ}C$):

45 (Lide 2003)

Boiling Point ($^{\circ}C$):

217.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.054 ($25^{\circ}C$, Biddiscombe et al. 1963)

1.011 ($25^{\circ}C$, Dean 1985)

Molar Volume (cm^3/mol):

147.8 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

10.0 (Dean 1985)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

50.84 (at normal boiling point, Biddiscombe et al. 1963)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

80.33 (at $25^{\circ}C$, Andon et al. 1960)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, $F: 0.636$ (mp at $45^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

24000* ($150^{\circ}C$, synthetic method-shake flask-optical, measured range 150 – $187^{\circ}C$, Erichsen & Dobbert 1955)

5000 (shake flask-spectrophotometry, Roberts et al. 1977)

7980 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($59.3^{\circ}C$, summary of literature data, temp range 59.3 – $219.0^{\circ}C$, Stull 1947)

9.67 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.55177 - 1943.1/(197.0 + t/^{\circ}C)$, temp range: 125 – $255^{\circ}C$, (Antoine eq. for liquid state, Dreisbach 1955)

1333* ($101.0^{\circ}C$, ebulliometry, measured range 101.0 – $218.2^{\circ}C$, Vonterres et al. 1955)

5.030 (calculated-Antoine eq., Biddiscombe et al. 1963)

4.96* ($25.03^{\circ}C$, ebulliometric and gas transpiration measurements, measured range 5 – $44^{\circ}C$, Biddiscombe et al. 1963)

$\log(P/mmHg) = 12.6090 - 4183.50/(t/^{\circ}C + 273)$; temp range 5 – $44^{\circ}C$ (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

$\log(P/mmHg) = 7.01297 - 1548.923/(t/^{\circ}C + 156.820)$; temp range 171 – $229^{\circ}C$ (Antoine eq. from ebulliometric and gas transpiration methods, Biddiscombe et al. 1963)

$\log (P/\text{mmHg}) = [-0.2185 \times 13437.9/(T/K)] + 8.854990$; temp range 59.3–219°C (Antoine eq., Weast 1972–73)
 6.575 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log (P/\text{kPa}) = 6.13614 - 1547.614/(156.677 + t/^\circ\text{C})$, temp range 171.8–229.1°C (Antoine eq. from reported exptl. data of Biddiscombe et al. 1963, Boublik et al. 1984)
 $\log (P/\text{kPa}) = 7.59041 - 2575.507/(242.273 + t/^\circ\text{C})$, temp range 101–218.2°C (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)
 7.530 (extrapolated-Antoine eq., Dean 1985)
 $\log (P/\text{mmHg}) = 8.291 - 2423/(229 + t/^\circ\text{C})$, temp range 101–218°C (Antoine eq., Dean 1985, 1992)
 4.95 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 11.74364 - 4188.624/(T/K)$, temp range 278–317 K, (Antoine eq.-I, solid, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.13939 - 1550.479/(-116.1 + T/K)$, temp range: 444–503 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)
 6.137 (extrapolated-four-parameter vapor pressure eq., Nesterova et al. 1990)
 $\log (P/\text{Pa}) = 96.72774 - 6779.787/(T/K) - 30.80658 \cdot \log (T/K) + 1.101581 \times 10^{-2} \cdot (T/K)$; temp range: 445–502 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)
 $\log (P/\text{mmHg}) = 16.9092 - 3.7255 \times 10^3/(T/K) - 1.7886 \cdot \log (T/K) - 4.2275 \times 10^{-3} \cdot (T/K) + 1.8002 \times 10^{-6} \cdot (T/K)^2$; temp range 318–716 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.132 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.75 (literature average, Leo et al. 1971)
 2.58 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
 2.26 (shake flask, Korenman 1972, Korenman et al. 1980)
 2.26, 2.58 (Hansch & Leo 1979)
 2.60 (shake flask-UV, Rogers & Wong 1980)
 2.37 (HPLC-RT correlation, Butte et al. 1981)
 2.12, 2.19 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 2.59 ± 0.07 ; 2.58 (HPLC-RV correlation-ALPM, selected best lit. value, Garst & Wilson 1984)
 2.50 (recommended, Sangster 1989, 1993)
 2.50 (COMPUTOX databank, Kaiser 1993)
 2.40; 2.58 (pH 7.4, pH 5.6, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.1.15.1
Reported aqueous solubilities of *p*-ethylphenol at various temperatures

Erichsen & Dobbert 1955	
synthetic method, SF-optical	
t/°C	S/g·m ⁻³
150	24000
160	30000
170	45000
180	93000
182	112000
184	141000
186	197000
187.1	395000

TABLE 14.1.1.15.2
Reported vapor pressures of *p*-ethylphenol at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log (P/mmHg) = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log (P/Pa) = A – B/(C + T/K)		(3)					
log (P/mmHg) = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Vonterres et al. 1955		Biddiscombe et al. 1963			
summary of literature data		ebulliometry		gas saturation		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
59.3	133.3	101.0	1333	5.0	0.480	171.757	26571
86.5	666.6	109.8	3333	10.0	0.907	178.525	33069
100.2	1333	137.5	6666	15.0	1.613	184.585	39942
115.0	2666	148.0	9999	19.99	2.813	189.724	46636
131.3	5333	155.5	13332	25.03	4.960	194.356	53416
141.7	7999	167.0	19998	30.02	8.426	198.419	59999
154.2	13332	177.2	26664	35.0	14.27	202.227	66736
175.0	26664	182.0	33330	39.99	23.33	205.607	73211
197.4	53329	187.7	39997	43.97	34.13	208.892	79979
219.0	101325	190.5	43330			211.911	86626
		192.6	46663			214.673	93090
mp/°C	46.5	197.0	53329	mp/°C	45.06	217.535	100174
		201.7	59995	bp/°C	217.985	220.026	106683
		204.0	66661			222.543	113599
		207.4	73327	for temp range:		224.769	119995
		210.9	79993	5–44°C		226.933	126484
		213.1	86659	eq. 2	P/mmHg	229.147	133418
		216.1	93325	A	12.6090		
		218.2	101325	B	4183.81	for temp range:	
				C	273	171–229°C	
						eq. 2	P/mmHg
				ΔH _v /(kJ mol ⁻¹)		A	7.01297
				at 25°C	80.33	B	1548.754
				at bp	50.84	C	156.820

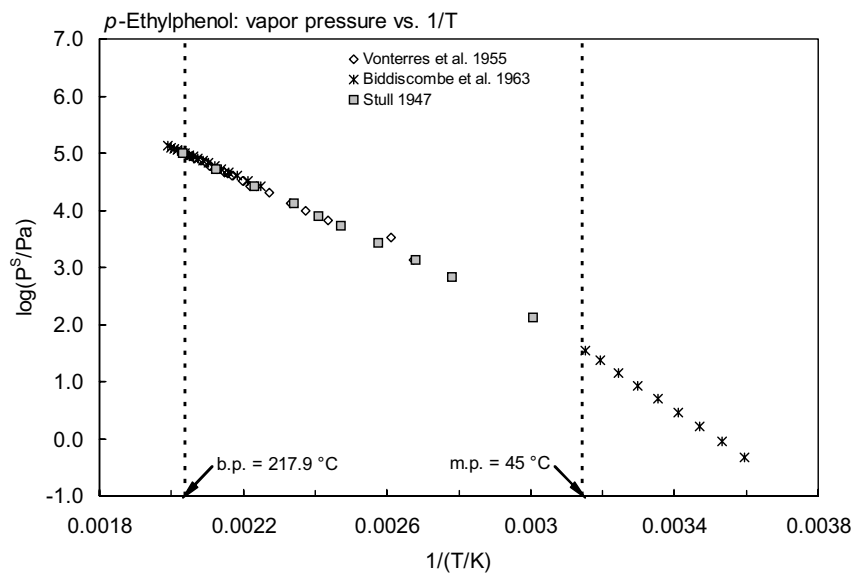
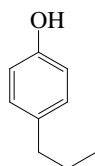


FIGURE 14.1.15.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-ethylphenol.

14.1.1.16 4-Propylphenol



Common Name: 4-Propylphenol

Synonym:

Chemical Name: 4-propylphenol

CAS Registry No: 645-56-7

Molecular Formula: $C_9H_{12}O$, $C_3H_7C_6H_4OH$

Molecular Weight: 136.190

Melting Point ($^{\circ}C$):

22 (West 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

232.6 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.009 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

170.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1278 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P_L/kPa) = 7.32632 - 2550.1/(-28.65 + T/K)$, temp range 383–508 K, (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.1 (HPLC-RT correlation, McLeese et al. 1979)

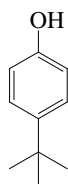
Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.1.17 *p*-*tert*-Butylphenol

Common Name: 4-*tert*-Butylphenol

Synonym: *p*-*tert*-butylphenol, 4-(α,α -dimethylethyl)phenol)

Chemical Name: 4-*tert*-butylphenol, *p*-*tert*-butylphenol

CAS Registry No: 98-54-4

Molecular Formula: $C_{10}H_{14}O$, $(CH_3)_3CC_6H_4OH$

Molecular Weight: 150.217

Melting Point ($^{\circ}C$):

98 (Lide 2003)

Boiling Point ($^{\circ}C$):

237 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

152.0 ($20^{\circ}C$, Stephenson & Malanowski 1987)

192.2 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

9.90 (McLeese et al. 1979)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

67.33, 50.62 ($25^{\circ}C$, bp, Dreisbach 1955)

50.54 (at normal boiling point, Handley et al. 1964)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.192 (mp at $98^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

650 (20 – $25^{\circ}C$, Geyer et al. 1981)

1000 (Thomas 1982)

700 (Verschueren 1983)

580 (Yalkowsky et al. 1987)

580 (shake flask-UV, Ahel & Giger 1993a)

1850 (shake flask-HPLC/UV at pH 6.05, Varhanířková et al. 1995)

753 (calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6.402* (extrapolated-regression of tabulated data, temp range 70 – $238^{\circ}C$, Stull 1947)

3.688 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/mmHg) = 7.49264 - 1999.8/(194.0 + t/^{\circ}C)$, temp range 140 – $370^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

1.225* (liquid, extrapolated-Antoine eq., ebulliometry, measured range 198 – $251^{\circ}C$, Handley et al. 1964)

$\log(P/mmHg) = 11.5638 - 3586.36/(t/^{\circ}C + 273)$; temp range 198 – $251^{\circ}C$ (Antoine eq. from ebulliometric measurements, Handley et al. 1964)

$\log(P/mmHg) = [-0.2185 \times 13787.7/(T/K)] + 8.785696$; temp range 70 – $238^{\circ}C$ (Antoine eq., Weast 1972–73)

5.072 (extrapolated-Cox eq., Chao et al. 1983)

$\log(P/mmHg) = [1 - 512.693/(T/K)] \times 10^4 \{0.834403 - 2.10918 \times 10^{-4} \cdot (T/K) + 0.554077 \times 10^{-7} \cdot (T/K)^2\}$; temp range 343.15 – $524.76 K$ (Cox eq., Chao et al. 1983)

1.24 (supercooled liquid P_L , extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/\text{kPa}) = 6.12365 - 1626.256/(155.092 + t/^{\circ}\text{C})$; temp range 198–231.6°C (Antoine eq. from reported exptl. data of Handley et al. 1964, Boublik et al. 1984)

1.25 (extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.00038 - 1627.51/(155.24 + t/^{\circ}\text{C})$, temp range 198–252°C (Antoine eq., Dean 1985, 1992)

1.272 (extrapolated-liquid, Antoine eq., Stephenson & Malanowski 1987)

0.492 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 11.46945 - 4405.873/(T/\text{K})$; temp range 280–304 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.13162 - 1632.939/(-117.258 + T/\text{K})$, temp range: 471–525 K, (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log (P/\text{Pa}) = 122.26679 - 8003.926/(T/\text{K}) - 40.16380 \cdot \log (T/\text{K}) + 1.40155 \times 10^{-2} \cdot (T/\text{K})$; temp range 471–525 K (four-parameter vapor pressure eq. derived using exptl data of Biddiscombe et al. 1963, Nesterova et al. 1990)

$\log (P/\text{mmHg}) = -54.7404 - 2.4727 \times 10^3/(T/\text{K}) + 28.991 \cdot \log (T/\text{K}) - 3.9356 \times 10^{-3} \cdot (T/\text{K}) + 1.543 \times 10^{-5} \cdot (T/\text{K})^2$; temp range 372–734 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

0.113 (calculated- $1/K_{AW}$, C_W/C_A , reported as exptl., Hine & Mookerjee 1975)

0.139; 3.750 (calculated-group contribution; calculated-bond contribution, Hine & Mookerjee 1975)

0.922 (calculated-P/C, Thomas 1982)

0.113, 0.375 (quoted, calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.04 (shake flask, Geyer et al. 1984)

2.94, 3.14 (shake flask-OECD 1981 Guideline, Geyer et al. 1984)

3.41 (HPLC-RT correlation, Butte et al. 1987)

3.04 (recommended, Sangster 1989)

3.31 (recommended, Hansch et al. 1995)

3.10 (HPLC-RT correlation, Makovskaya et al. 1995b)

2.95 (solid-phase microextraction, Dean et al. 1996)

Bioconcentration Factor, $\log \text{BCF}$:

1.53 (*Chlorella*, after exposure to 50 $\mu\text{g}/\text{L}$ for 24 h, Geyer et al. 1981)

1.88 (calculated-S, Geyer et al. 1981)

1.53; 2.08 (algae, golden *orfe*, Freitag et al. 1982)

2.38 (activated sludge, Freitag et al. 1982, 1985)

1.53 (Alga *Chlorella fusca*, wet weight basis, Geyer et al. 1984)

1.48; 2.07 (algae; golden ide, Freitag et al. 1985)

1.86 (zebrafish, Butte et al. 1987; quoted, Devillers et al. 1996)

2.38; 1.48; 2.07 (activated sludge; algae; fish; Freitag et al. 1987)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: volatilization

$t_{1/2} = 117$ h from water body with depth of 1 m (Thomas 1982).

Half-Lives in the Environment:

TABLE 14.1.1.17.1

Reported vapor pressures of *p*-*tert*-butylphenyl at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \quad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \quad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Stull 1947		Handley et al. 1964			
summary of literature data		ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
70.0	133.3	198.21	33059	mp/°C	99.55
99.2	666.6	204.527	39955	bp/°C	239.83
114	1333	209.901	46592	for temp range: 198–251°C	
129.5	2666	214.892	53489		
146	5333	219.142	59984	eq. 2	P/mmHg
156	7999	223.088	66579	A	6.99455
170.2	13332	226.818	73350	B	1623.046
191.5	26664	230.203	79963	C	154.716
214	53329	233.457	86724	$\Delta H_v/(\text{kJ mol}^{-1})$	
238	101325	236.342	92123	at bp	50.54
		239.305	100052		
mp/°C	99.0	242.180	106758		
		244.560	113369		
		247.015	120049		
		249.336	126634		
		251.608	133354		

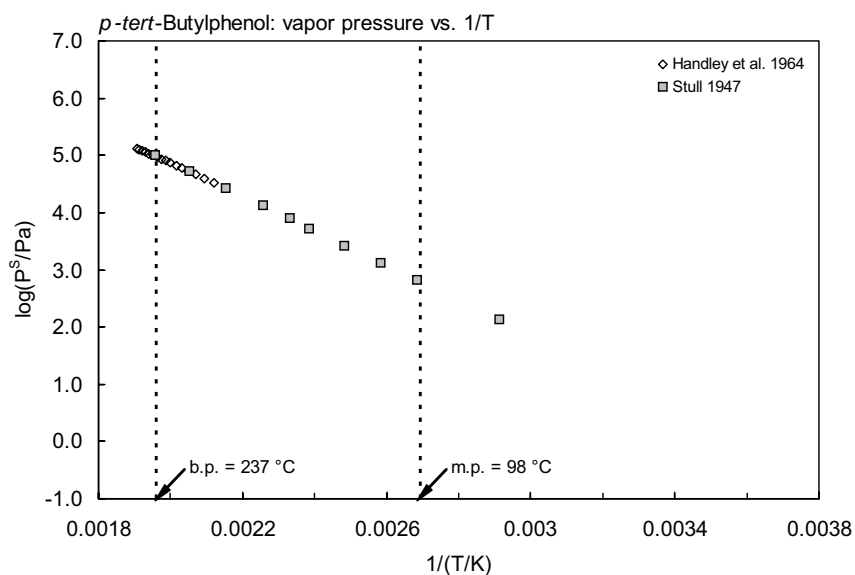
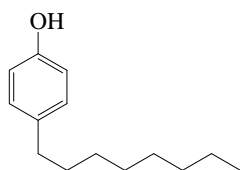


FIGURE 14.1.1.17.1 Logarithm of vapor pressure versus reciprocal temperature for *p*-*tert*-butylphenol.

14.1.1.18 4-Octylphenol



Common Name: 4-Octylphenol

Synonym: *p*-octylphenol

Chemical Name: 4-octylphenol

CAS Registry No: 27193-28-8

Molecular Formula: $C_{14}H_{22}O$, $C_8H_{17}-C_6H_4OH$

Molecular Weight: 206.324

Melting Point ($^{\circ}C$):

43 (Lide 2003)

Boiling Point ($^{\circ}C$):

280-283 (Lewis 1996)

Density (g/cm^3 at $20^{\circ}C$):

0.941 (at $24^{\circ}C$, Lewis 1996)

Molar Volume (cm^3/mol):

281.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.666 (mp at $43^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

12.6 ± 0.50 (generator column-HPLC/fluor., Ahel & Giger 1993a)

14.1 ± 0.60 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

0.071 (quoted, Shiu et al. 1994)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.4916 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.70 (calculated- π substituent const. or fragment const., McLeese et al. 1981)

4.12 ± 0.10 (shake flask-HPLC/fluor., Ahel & Giger 1993b)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

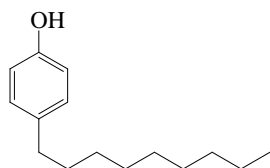
Biodegradation: average exptl. rate constant $k = 0.0894 h^{-1}$ compared to group contribution method predicted rate constants $k = 0.1124 h^{-1}$ (nonlinear) and $k = 0.0982 h^{-1}$ (Tabak & Govind 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

14.1.1.19 4-Nonylphenol



Common Name: 4-Nonylphenol

Synonym: *p*-nonylphenol

Chemical Name: 4-nonylphenol

CAS Registry No: 104-40-5; 25154-52-3

Molecular Formula: $C_{15}H_{24}O$, $C_9H_{19}C_6H_4OH$

Molecular Weight: 220.351

Melting Point ($^{\circ}C$):

42 (Lide 2003)

Boiling Point ($^{\circ}C$):

approx. 295 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.513 (Budavari 1989)

Molar Volume (cm^3/mol):

231.1 ($20^{\circ}C$, Stephenson & Malanowski 1987)

303.2 (calculated-Le Bas method at normal boiling)

Acid Dissociation Constant, pK_a :

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F : 0.681 (mp at $42^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5.43 ± 0.17 (generator column-HPLC/fluor., Ahel & Giger 1993a)

4.90 ± 0.4 (shake flask-GC/FID, Brix et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.0701* (ebulliometry, extrapolated, measured range 214.78 – $321.91^{\circ}C$, Hon et al. 1976)

$\log (P/mmHg) = 7.74950 - 2550.67/(260.28 + t/^{\circ}C)$; temp range 214.78 – $321.91^{\circ}C$ (Antoine eq., ebulliometry, Hon et al. 1976)

0.0720 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 6.8847 - 2560.53/(207.199 + t/^{\circ}C)$, temp range 214.8 – $321.8^{\circ}C$ (Antoine eq. from reported exptl. data of Hon et al. 1976, Boublik et al. 1984)

0.0691 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 6.87147 - 2547.289/(-67.246 + T/K)$, temp range 487 – $595 K$ (Antoine eq., Stephenson & Malanowski 1987)

0.174, 0.14, 0.109, 0.0908, 0.0802, 0.0556 (GC-RT correlation, 7 isomers, Bidleman & Renberg 1985)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

1.5705 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.20 (calculated- π substituent const. or fragment const., McLeese et al. 1981)

4.10 (Geyer et al. 1982)

5.90 (selected, Yoshida et al. 1986)

5.76 (HPLC-RT correlation, Itokawa et al. 1989)

4.48 ± 0.12 (shake flask-HPLC/fluor., Ahel & Giger 1993b)

6.36 (calculated-CLOGP 3.51, Jaworska & Schultz 1993)

- 6.36 (COMPUTOX, Kaiser 1993)
 5.76 (Sangster 1993; Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 2.45 (salmon, McLeese et al. 1981)
 1.00 (mussel *mytilus edulis*, Geyer et al. 1982)
 2.40 (fish liver, Ahel & Giger 1993a)
 2.22; 2.45 (laboratory BCF data: killifish; salmon; Tsuda et al. 2000)
 1.49; 1.32; 1.40; 1.34; 1.32; 1.18; 1.11–2.61 (field BCF data: pale chub; Ayu sweetfish, dark chub, crucian carp; large-mouth bass; bluegill; fish tissue; Tsuda et al. 2000)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Biodegradation: average exptl. rate constant of 0.0894 h^{-1} compared to group contribution method predicted rate constants of 0.1124 h^{-1} (nonlinear) and 0.0982 h^{-1} (linear) (Tabak & Govind 1993).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 45.0 \text{ d}^{-1}$ (McLeese et al. 1981)

$k_2 = 0.16 \text{ d}^{-1}$ (McLeese et al. 1981)

Half-Lives in the Environment:

Biota: $t_{1/2} = 4 \text{ d}$ in salmon before excretion (McLeese et al. 1981).

TABLE 14.1.1.19.1
Reported vapor pressures of 4-nonylphenol at various temperatures

Hon et al. 1976	
ebulliometry	
$t/^{\circ}\text{C}$	P/Pa
214.78	6557
251.33	19998
261.87	26679
274.76	37250
283.74	46663
289.28	53364
298.78	66656
303.76	74873
307.72	81628
310.82	87441
314.17	94271
317.1	100170
321.81	110655
bp/ $^{\circ}\text{C}$	317.61

(Continued)

TABLE 14.1.1.19.1 (*Continued*)**Hon et al. 1976****ebulliometry****t/°C** **P/Pa** $\log P = A - B/(C + t/^{\circ}\text{C})$

P/mmHg

A 7.74950

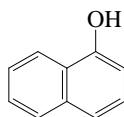
B 2550.67

C 260.28

 $\Delta H_v/(\text{kJ mol}^{-1})$

at bp 61.923

14.1.1.20 1-Naphthol



Common Name: 1-Naphthol

Synonym: α -naphthol, 1-naphthalenol, 1-hydroxynaphthalene

Chemical Name: 1-naphthol

CAS Registry No: 90-15-3

Molecular Formula: $C_{10}H_8O$, $C_{10}H_7OH$

Molecular Weight: 144.170

Melting Point ($^{\circ}C$):

95 (Lide 2003)

Boiling Point ($^{\circ}C$):

288.0 (sublimation, Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm^3):

1.0989 ($99^{\circ}C$, Weast 1982–83)

1.0954 ($99^{\circ}C$, Dean 1985)

Acid Dissociation Constant, pK_a :

9.20 (McLeese et al. 1979)

9.30 (Dean 1985)

Molar Volume (cm^3/mol):

131.2 ($99^{\circ}C$, Stephenson & Malanowski 1987)

155.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

23.47 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

63.6 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$, F: 0.206 (mp at $95^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

438 (quoted, Tsonopoulos & Prausnitz 1971)

870; 674 (exptl., calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.550* (extrapolated-regression of tabulated data, temp range 94 – $282.5^{\circ}C$, Stull 1947)

1333* ($141.5^{\circ}C$, ebulliometry, measured range 141.5 – $282.5^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 14205.6/(T/K)] + 8.476669$; temp range 94 – $282.5^{\circ}C$ (Antoine eq., Weast 1972–73)

0.509 (extrapolated-liquid, Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.69308 - 2275.566/(202.869 + t/^{\circ}C)$, temp range 141.5 – $282.5^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

0.290 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.28421 - 2077.56/(184.0 + t/^{\circ}C)$; temp range 141 – $282^{\circ}C$ (Antoine eq., Dean 1985, 1992)

$\log(P_s/kPa) = 12.20753 - 4873.394/(T/K)$; temp range 298 – $312\ K$ (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.70115 - 4405.522/(T/K)$; temp range 314 – $324\ K$ (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.53825 - 3083.8/(1.731 + T/K)$; temp range 399 – $556\ K$ (Antoine eq.-III, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.49 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.98	(shake flask-UV, Hansch & Anderson 1967)
2.98, 2.84, 2.31	(Hansch & Leo 1979)
2.28	(HPLC- k' correlation, Haky & Young 1984)
2.84	(recommended, Sangster 1989, 1993)
2.84	(CPC centrifugal partition chromatography, Gluck & Martin 1990)
3.13	(back-flushing-CPC centrifugal partition chromatography, Menges et al. 1990)
2.81	(shake flask-HPLC, Menges et al. 1991)
3.02	(concurrent chromatography, Berthod et al. 1988)
2.84	(COMPUTOX, Kaiser 1993)
2.43	(HPLC-RT correlation, Ritter et al. 1994)
2.84	(recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:Bioconcentration Factor, $\log BCF$:Sorption Partition Coefficient, $\log K_{OC}$:

2.64	(soil and sediment, Hassett et al. 1981)
3.33	(soil, Means et al. 1982)
3.41	(soil, calculated-MCI χ , Sabljic 1987)
2.10–2.77	(soil, calculated- K_{ow} , model of Karickhoff et al. 1979, Sabljic 1987)
2.63–2.99	(soil, calculated- K_{ow} , model of Kenaga & Goring 1980, Sabljic 1987)
1.84–2.1	(soil, calculated- K_{ow} , model of Briggs 1981, Sabljic 1987)
1.99–2.66	(soil, calculated- K_{ow} , model of Means et al. 1982, Sabljic 1987)
1.30–1.90	(soil, calculated- K_{ow} , model of Chiou et al. 1983, Sabljic 1987)
2.89	(soil, calculated-MCI χ , Bahnick & Doucette 1988)
2.52–2.96, 2.53	(soil: quoted, calculated- K_{ow} , Xing et al. 1994)
1.92–2.64	(organic sorbent: cellulose, lignin, Xing et al. 1994)
3.31, 2.91, 2.61	(RP-HPLC- k' correlation on 3 different stationary phases, Szabo et al. 1995)
2.61; 3.48	(HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)

Environmental Fate Rate Constants, k and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation 38.4 mg COD $g^{-1} \cdot h^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

TABLE 14.1.1.20.1
Reported vapor pressures of 1-naphthol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
94.0	133.3	141.5	1333
125.5	666.6	164.8	3333
142	1333	184.2	6666
158	2666	196.9	9999
177.8	5333	206.0	13332
190	7999	219.3	19998
206	13332	229.0	26664
229.6	26664	236.4	33330
255.8	53329	244.0	39997
282.5	101325	246.5	43330
		250.2	46663
mp/°C	96.0	255.1	53329
		260.3	59995
		264.8	66661
		265.7	73327
		272.0	79993
		275.2	86659
		278.3	93325
		282.5	101325

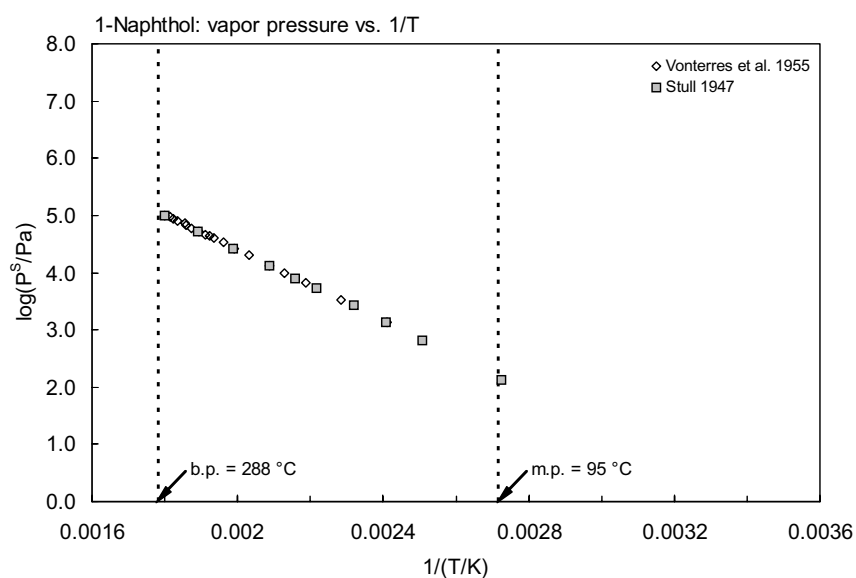
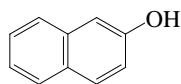


FIGURE 14.1.1.20.1 Logarithm of vapor pressure versus reciprocal temperature for 1-naphthol.

14.1.1.21 2-Naphthol



Common Name: 2-Naphthol

Synonym: β -naphthol, 2-naphthalenol, 2-hydroxynaphthalene

Chemical Name: 2-naphthol

CAS Registry No: 135-19-3

Molecular Formula: $C_{10}H_7OH$

Molecular Weight: 144.170

Melting Point ($^{\circ}C$):

121.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.280 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.57 (Dean 1985)

Molar Volume (cm^3/mol):

155.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

18.79 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

47.7 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$), F: 0.113 (mp at $121.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

680* ($23.20^{\circ}C$, shake flask, measured range 15.55–31.25, McCune & Wilhelm 1949)

700 (20 – $25^{\circ}C$, Seidell 1941; Lange 1973)

713* ($21.5^{\circ}C$, shake flask-UN spectrophotometry, measured range 6.9 – $75^{\circ}C$, Moyle & Tyner 1953)

754 (Tsonopoulos & Prausnitz 1971)

1000 (shake flask-UV spectrophotometry, Roberts et al. 1977)

740 (Verschuereen 1983)

477 (calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1.430* (extrapolated-regression of tabulated data, temp range 128.5 – 288° , Stull 1947)

1333* ($144.0^{\circ}C$, ebulliometry, measured range 144.0 – $288.0^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 14138.5/(T/K)] + 8.391271$; temp range 128.6 – $288^{\circ}C$ (Antoine eq., Weast 1972–73)

0.386 (extrapolated-Antoine eq., supercooled liquid P_L , Boublik et al. 1984)

$\log(P/kPa) = 6.62476 - 2244.555/(198.594 + t/^{\circ}C)$, temp range 144 – $288^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

0.160 (extrapolated-Antoine eq., supercooled liquid P_L , Dean 1985)

$\log(P/mmHg) = 7.34714 - 2135.0/(183.0 + t/^{\circ}C)$, temp range 144 – $288^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.0303 (interpolated-Antoine eq.-III, solid P_s , Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 12.48704 - 5110.333/(T/K)$, temp range 298 – $312\ K$ (Antoine eq.-I, α form, solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 10.80636 - 4586.029/(T/K)$, temp range 314 – $332\ K$ (Antoine eq.-II, β form, solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 9.273 - 4112/(T/K)$, temp range 283 – $323\ K$ (Antoine eq.-III, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.22927 - 2827.5/(-19.868 + T/K)$, temp range 401 – $561\ K$ (Antoine eq.-IV, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.280 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

2.84 (shake flask-UV, Hansch & Anderson 1967)
 2.70, 2.84, 2.89 (Hansch & Leo 1979)
 2.01, 2.46 (HPLC- k' correlation, Eadsforth 1986)
 2.84 (recommended, Sangster 1989)
 2.85 (centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)
 2.70 (EPA CLOGP Data Base, Hulzebos et al. 1993)
 2.70 (COMPUTOX, Kaiser 1993)
 2.70 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.33 (soil, Means et al. 1982)
 3.41 (soil, calculated-MCI χ , Sabljic 1987)
 2.10–2.77 (soil, calculated- K_{OW} based on model of Karickhoff et al. 1979, Sabljic 1987)
 2.63–2.99 (soil, calculated- K_{OW} based on model of Kenaga & Goring 1980, Sabljic 1987)
 1.84–2.19 (soil, calculated- K_{OW} based on model of Briggs 1981, Sabljic 1987)
 1.99–2.66 (soil, calculated- K_{OW} based on model of Means et al. 1982, Sabljic 1987)
 1.30–1.90 (soil, calculated- K_{OW} based on model of Chiou et al. 1983, Sabljic 1987)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: average rate of biodegradation $39.2 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 14.1.1.21.1

Reported aqueous solubilities and vapor pressures of 2-naphthol at various temperatures

Aqueous solubility				Vapor pressure			
McCune & Wilhelm 1949		Moyle & Tyner 1953		Stull 1947		Vonterres et al. 1955	
shake flask		shake flask-UV spec.		summary of literature data		ebulliometry	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa
15.55	501	6.90	355	128.6	666.6	144.0	1333
16.24	526	13.45	487	145.5	1333	158.0	3333
23.20	680	17.7	561	161.8	2666	188.0	6666
31.25	928	21.5	713	181.7	5333	200.5	9999
		29.5	876	193.7	7999	210.0	13332
		33.3	985	209.8	13332	223.1	19998
log (100·C _w) = A – B/(T/K)		38.7	1304	234.0	26664	233.0	26664
C _w	g/100 mL	44.5	1609	260.6	53329	246.0	33330
A	5.8833	48.5	2001	288.0	101325	247.4	39997
B	1495.84	55.2	2460			251.0	43330
		60.0	3034	mp/°C	122.5	254.2	46663
		68.1	4222			260.2	53329
		75.0	5493			265.1	59995
						269.0	66661
						273.0	73327
						276.6	79993
						279.7	86659
						283.0	93325
						288.0	101325

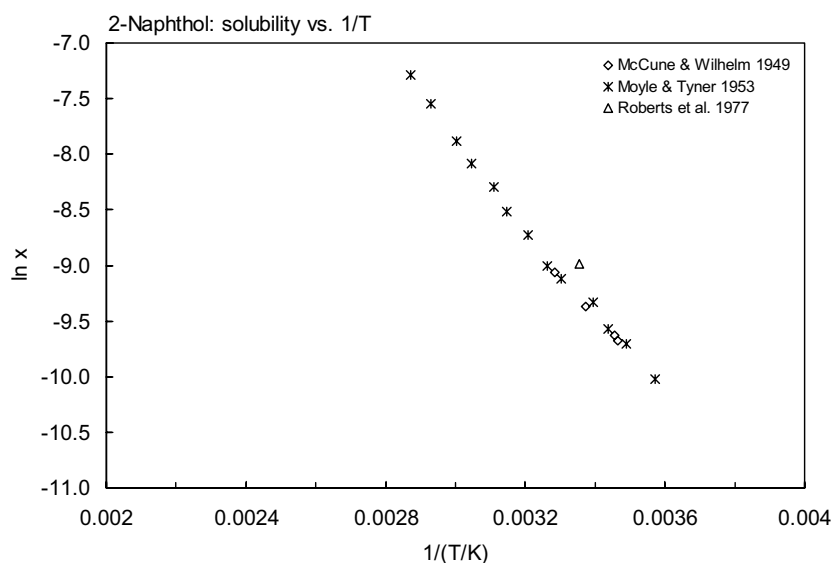


FIGURE 14.1.1.21.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 2-naphthol.

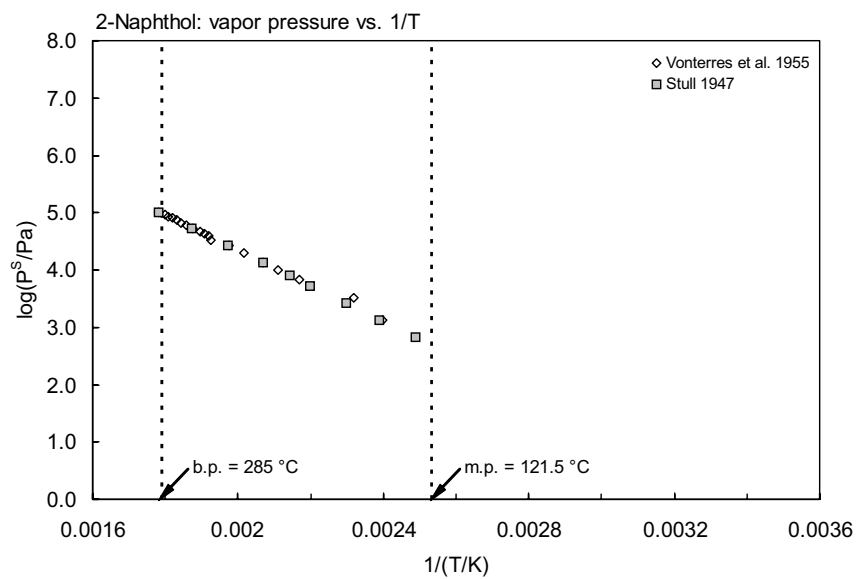
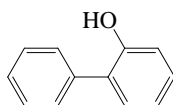


FIGURE 14.1.1.21.2 Logarithm of vapor pressure versus reciprocal temperature for 2-naphthol.

14.1.1.22 2-Phenylphenol (2-Hydroxybiphenyl)



Common Name: 2-Phenylphenol

Synonym: *o*-phenylphenol, 2-hydroxybiphenyl, [1,1'-biphenyl]-2-ol

Chemical Name: 2-phenylphenol

CAS Registry No: 90-43-7

Molecular Formula: $C_{12}H_{10}O$, $C_6H_5C_6H_4OH$

Molecular Weight: 170.206

Melting Point ($^{\circ}C$):

57.5 (Weast 1982–83)

Boiling Point ($^{\circ}C$):

286 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.213 (Dean 1985)

1.200 ($25^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

192.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

9.55 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.480 (mp at $57.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

700 (Verschueren 1983)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($100^{\circ}C$, summary of literature data, temp range 100 – $275^{\circ}C$, Stull 1947)

1333* ($161.9^{\circ}C$, ebulliometry, measured range 161.9 – $275.0^{\circ}C$, Vonterres et al. 1955)

$\log (P/mmHg) = [-0.2185 \times 15397.8/(T/K)] + 9.015370$; temp range 100 – $275^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log (P/mmHg) = [1 - 549.249/(T/K)] \times 10^4 \{0.889463 - 4.72320 \times 10^{-4} \cdot (T/K) + 5.27654 \times 10^{-7} \cdot (T/K)^2\}$; temp range 373.15 – $548.15 K$ (Cox eq., Chao et al. 1983)

2667, 13330 ($163^{\circ}C$, $206^{\circ}C$, Verschueren 1983)

$\log (P/kPa) = 5.50723 - 1137.035/(72.282 + t/^{\circ}C)$, temp range 161.9 – $275^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

30.0 (interpolated-Antoine eq.-I, solid P_s , Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 10.8635 - 4326.754/(T/K)$, temp range 291 – $314 K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 4.1553 - 547.8/(-298.55 + T/K)$, temp range 434 – $547 K$ (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.09 (Hansch & Leo 1979)

3.09 (COMPUTOX, Kaiser 1993)

3.06 (HPLC-RT correlation, Ritter et al. 1994)

3.09 (recommended, Sangster 1993)

3.06 (HPLC-RT correlation, Ritter et al. 1994)

3.09 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 66\text{--}3840$ h in water, based on reported reaction rate constants for OH and RO_2 radicals to react with phenol class compounds (Mill & Mabey 1985; Guesten et al. 1981; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 0.1\text{--}22$ h, based on estimated reaction rate constant with OH radical (Atkinson 1987; quoted, Howard et al. 1991) and NO_3 radical in nighttime air to react with the phenol and cresol classes (Howard et al. 1991).

Hydrolysis:

Biodegradation: 100% degradation under aerobic and anaerobic conditions after 3 wk (504 h) at 22°C (Verschuereen 1983);

$t_{1/2}$ (aq. aerobic) = 24–168 h, based on a river die-away study in which a 50% degradation was observed over a one week period (Gonsior et al. 1984; quoted, Howard et al. 1991); $t_{1/2}$ (aq. anaerobic) = 96–672 h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 0.1\text{--}22$ h, based on estimated reaction rate constant with OH radical (Atkinson 1987; quoted, Howard et al. 1991) and NO_3 radical in nighttime air to react with the phenol and cresol classes (Howard et al. 1991).

Surface water: photooxidation $t_{1/2} = 66\text{--}3840$ h in water, based on reported reaction rate constants for OH and RO_2 radicals to react with phenol class compounds (Mill & Mabey 1985; Güesten et al. 1981; quoted, Howard et al. 1991); $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 14.1.1.22.1
Reported vapor pressures of 2-phenylphenol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
100	133.3	161.9	1333
131.6	666.6	168.0	3333
146.2	1333	188.1	6666
163.3	2666	198.0	9999
180.3	5333	206.8	13332
192.2	7999	219.0	19998
205.9	13332	228.1	26664
227.9	26664	235.2	33330
251.8	53329	241.6	39997
275.0	101325	244.0	43330
		247.4	46663

(Continued)

TABLE 14.1.1.22.1 (Continued)

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
mp/°C	56.6	252.0	53329
		257.0	59995
		261.0	66661
		264.0	73327
		268.0	79993
		270.0	86659
		273.8	93325
		275.0	101325
		bp/°C	278.004

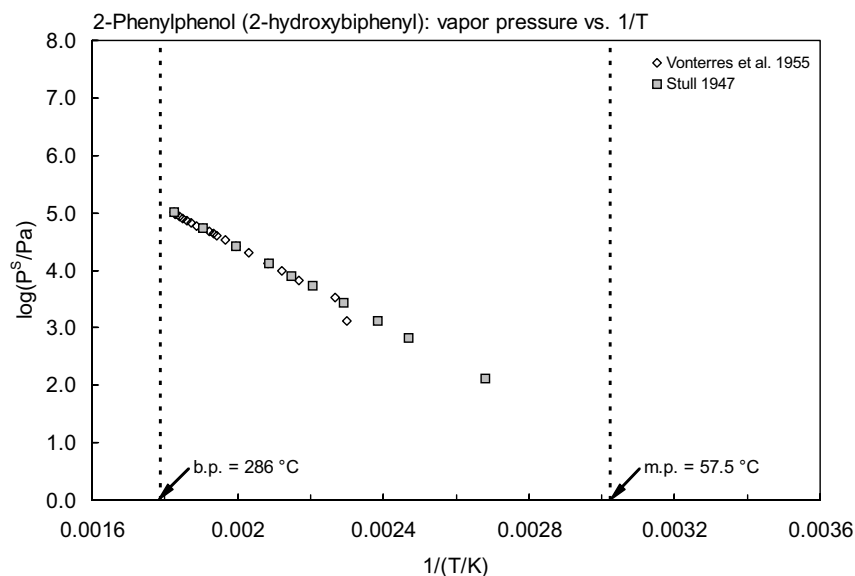
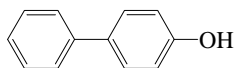


FIGURE 14.1.1.22.1 Logarithm of vapor pressure versus reciprocal temperature for 2-phenylphenol.

14.1.1.23 4-Phenylphenol (4-Hydroxybiphenyl)



Common Name: 4-Phenylphenol

Synonym: *p*-phenylphenol, 4-hydroxybiphenyl, [1,1'-biphenyl]-4-ol

Chemical Name: 4-phenylphenol

CAS Registry No: 92-69-3

Molecular Formula: $C_{12}H_{10}O$, $C_6H_5C_6H_4OH$

Molecular Weight: 170.206

Melting Point ($^{\circ}C$):

166 (Lide 2003)

Boiling Point ($^{\circ}C$):

305–308 (sublimation, Weast 1982–83; Stephenson & Malanowski 1987)

305 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

192.0 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

9.55 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.0414 (mp at $166^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9.79 (CESARS 1988)

56.4; 50.2 (quoted exptl.; calculated-group contribution, Kühne et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

1333* ($176.2^{\circ}C$, summary of literature data, temp range 176.2 – $308^{\circ}C$, Stull 1947)

1333* ($177.0^{\circ}C$, ebulliometry, measured range 177.0 – $308.0^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 16974.3/(T/K)] + 9.234838$; temp range 176.2 – $308^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [1 - 580.171/(T/K)] \times 10^{\{0.949514 - 5.554686 \times 10^{-4} \cdot (T/K) + 5.61184 \times 10^{-7} \cdot (T/K)^2\}}$; temp range: 450.15 – $581.15 K$, (Cox eq., Chao et al. 1983)

0.0278 (liquid, extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.97182 - 3214.349/(231.575 + t/^{\circ}C)$, temp range 177 – $308^{\circ}C$ (Antoine eq. from reported exptl. data of Vonterres et al. 1955, Boublik et al. 1984)

0.020 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 8.6575 - 3022.8/(216.1 + t/^{\circ}C)$; temp range: 177 – $308^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.00153 (extrapolated-Antoine eq., solid P_s , Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 11.17513 - 5066.004/(T/K)$; temp range 327 – $348 K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.41978 - 3684.9/(-5.81 + T/K)$, temp range 450 – $581 K$ (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.20 (shake flask-UV, Norrington et al. 1975)

3.63 (HPLC-RV correlation, Garst 1984)

2.88 (centrifugal partition chromatography (CPC), Terada et al. 1987)

3.20 (COMPUTOX databank, Kaiser 1993)

3.31 (HPLC-RT correlation, Ritter et al. 1994)

3.20 (recommended, Sangster 1993)

3.20 (recommended, Hansch et al. 1995)

2.60, 2.56, 2.70, 2.72 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

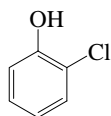
TABLE 14.1.1.23.1

Reported vapor pressures of 4-phenylphenol at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
176.2	1333	177.0	1333
193.8	2666	199.2	3333
213.0	5333	217.8	6666
225.3	7999	229.0	9999
240.9	13332	237.4	13332
263.2	26664	250.0	19998
285.5	53329	260.2	26664
308.0	101325	267.1	33330
		273.8	39997
mp/ $^{\circ}\text{C}$	164.5	276.0	43330
		278.8	46663
		283.0	53329
		287.1	59995
		291.0	66661
		294.7	73327
		297.8	79993
		300.6	86659
		303.5	93325
		308.0	101325
		bp/ $^{\circ}\text{C}$	307.194

14.1.2 CHLOROPHENOLS

14.1.2.1 2-Chlorophenol



Common Name: 2-Chlorophenol

Synonym: *o*-chlorophenol, 1-chloro-2-hydroxybenzene

Chemical Name: 2-chlorophenol

CAS Registry No: 95-57-8

Molecular Formula: $C_6H_4(OH)Cl$

Molecular Weight: 128.556

Melting Point ($^{\circ}C$):

9.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

174.9 (Dreisbach 1955; Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.2634 ($20^{\circ}C$, Weast 1982–83)

1.257 ($25^{\circ}C$, Krijghsheld & van der Gen 1986)

Acid Dissociation Constant, pK_a :

8.65 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

8.48 (Pearce & Simkins 1968; Krijghsheld & van der Gen 1986)

8.52 (Drahonovsky & Vacek 1971)

8.29 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)

8.55 (Serjeant & Dempsey 1979)

8.30 (Hoigné & Bader 1983)

9.30 (HPLC, Miyake et al. 1987)

Molar Volume (cm^3/mol):

101.8 ($20^{\circ}C$, Stephenson & Malanowski 1987)

124.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.05, 49.25 (normal bp, $25^{\circ}C$, Dreisbach 1955)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

13.50 (Dreisbach 1955)

10.75 (Tsonopoulos & Prausnitz 1971)

12.52 (Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

38.12 (Tsonopoulos & Prausnitz 1971)

44.24 (exptl., Chickos et al. 1999)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

25000* ($20^{\circ}C$, synthetic method, measured range -0.20 to $173.0^{\circ}C$, Sidgwick & Turner 1922)

29000 (20 – $25^{\circ}C$, Seidell 1941; Urano et al. 1982)

24650 ($20^{\circ}C$, shake flask-UV, Mully & Metcalf 1966)

22000 (shake flask-spectrophotometry, Roberts et al. 1977)

28500 ($20^{\circ}C$, Verschueren 1977, 1983)

11480 (shake flask-LSC, Banerjee et al. 1980)

11200 (shake flask-radioactive analysis, Veith et al. 1980)

20000 (recommended, IUPAC Solubility Data Series, Horvath & Getzen 1985)

23260 (shake flask-HPLC/UV at pH 4.8, Ma et al. 1993)

28500 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

22660* (24.6°C, shake flask-conductimetry, measured range 15.4–34.5°C, Achard et al. 1996)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

316* (interpolated-regression of tabulated data, temp range 12.7–174.5°C, Stull 1947)

208 (calculated-Antoine eq., Dreisbach 1955)

$\log(P/\text{mmHg}) = 7.05272 - 1589.1/(206.0 + t/^{\circ}\text{C})$, temp range 80–300°C (Antoine eq. for liquid state, Dreisbach 1955)

313 (extrapolated from Antoine eq., Weast 1972–73)

$\log(P/\text{mmHg}) = [-0.2185 \times 10341.1/(T/K)] + 7.952334$; temp range 12.1–174.5°C (Antoine eq., Weast 1972–73)

5532 (80°C, Verschueren 1977, 1983)

293, 180.7 (extrapolated, Antoine eq., Dean 1985)

$\log(P/\text{mmHg}) = 6.87731 - 1471.61/(193.17 + t/^{\circ}\text{C})$; temp range 80–200°C (Antoine eq., Dean 1985, 1992)

131.8 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.78693 - 1314.9/(-101.95 + T/K)$, temp range 333–449 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 5.3685 - 1096.98/(-122.58 + T/K)$; temp range 354–448 K (Antoine eq.-II, Stephenson & Malanowski 1987)

737, 1329, 2278, 3736, 5907 (50, 60.24, 69.94, 79.95, 89.94°C, calculated-Antoine eq. of Stephenson & Malanowski 1987, Tabai et al. 1997)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

1.065 (calculated-P/C, Mabey et al. 1982)

0.688 (calculated-P/C, Shiu et al. 1994)

0.661 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

$k_H/\text{kPa} = 161.250 - 12658.0/(T/K) - 20.4027$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.15 (shake flask-UV, Fujita et al. 1964;)

2.15, 2.19 (Leo et al. 1971)

2.20 (calculated using data from Fujita et al. 1964, Umeyama et al. 1971)

2.12 (20°C, shake flask, Korenman 1974)

2.15 (LC- k' correlation, Carson et al. 1975)

2.17 (Hansch & Leo 1979)

2.16 (shake flask-LSC, Banerjee et al. 1980)

0.83 (RP-HPLC-RT correlation, Veith et al. 1980)

2.11 (RP-HPLC-RT correlation, Butte et al. 1981)

2.03 (shake flask, Dearden & Bresnen 1981)

2.16 ± 0.03 (HPLC- k' correlation, Hammers et al. 1982)

2.32 (RP-HPLC-RT correlation, Chin et al. 1986)

1.56, 1.99 (HPLC- k' correlation, Eadsforth 1986)

2.09 (HPLC-RT correlation, Miyake et al. 1986)

2.13 (shake flask-UV, Miyake et al. 1987)

2.16 (shake flask-CPC, Berthod et al. 1988)

2.24 (batch equilibration-UV, Beltrame et al. 1988)

2.11 (centrifugal partition chromatography, Gluck & Martin 1990)

2.25 (back flashing-CPC centrifugal partition chromatography; Menges et al. 1990)

2.05 (centrifugal partition chromatography CPC-RV, El Tayar et al. 1991)

2.17 (counter-current chromatography, Berthod et al. 1992)

2.15 (recommended, Sangster 1993)

2.29 (shake flask-GC, Kishino & Kobayashi 1994)

2.15 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

2.33	(bluegill sunfish, Barrows et al. 1980)
2.33	(bluegill sunfish, Veith et al. 1980)
1.61	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
2.33	(bluegill sunfish, Bysshe 1982)
0.81	(gold fish, Kobayashi et al. 1979; quoted, Verschueren 1983; Howard 1989)
0.81	(Isnard & Lambert 1988)
0.28–1.40	(estimated from K_{OW} , Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

3.70, 3.60	(sediment: fine, coarse; Isaacson & Frink 1984)
1.86	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
1.71	(clay loam soil, Boyd 1982; quoted, Howard 1989)
3.69	(untreated fine sediment, Isaacson & Frink 1984)
3.60	(untreated coarse sediment, Isaacson & Frink 1984)
3.98	(treated fine sediment, Isaacson & Frink 1984)
4.36	(treated coarse sediment, Isaacson & Frink 1984)
1.20–2.55	(estimated from K_{OW} , Howard 1989)
1.82	(calculated- K_{OW} , Kollig 1993)
2.60	(soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.35, 1.60$ h from stirred and static water at 23.8°C (Chiou et al. 1980; Howard 1989);
 $t_{1/2} = 73$ d, based on estimation from a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1989).

Photolysis: vapor phase $t_{1/2} = 47$ h (Howard 1989);

first-order photolysis disappearance rate constant $k = 3.01 \times 10^{-2} \text{ min}^{-1}$ in the absence of DOM at 313 nm (Kawaguchi 1992).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(aq.) < 7 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $1 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k(aq.) = 66 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, $k = (1.1 \pm 0.3) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k = (0.2 \pm 0.1) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.8–4 and 20–23°C (Hoigné & Bader 1983b)

$k_{OH} = 1.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in air (Bunce et al. 1991)

$k(aq.) = (9.2 \pm 9.4) \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991)

Hydrolysis:

Biodegradation: average rate $k = 25.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mL in 14–25 d by wastewater (Haller 1978);

aerobic degradation in a non-sterile clay loam soil: 91% loss at 0°C after 8 d at the termination of the experiment, 94% loss at 4°C after 8 d and 100% loss at 20°C after 10–15 d all under same exptl. conditions (Baker et al. 1980);

rate constants $k = 1.0 \text{ d}^{-1}$ with $t_{1/2} = 0.7$ d in adopted activated sludge and $k = 0.3 \text{ d}^{-1}$ with $t_{1/2} = 2.3$ d in soil suspension under aerobic conditions (Mills et al. 1982);

completely degraded in soil suspensions in 14 d and by a soil microflora within 64 d (quoted, Verschueren 1983);

approximately 48 h in a column microcosm under aerobic conditions (Sufliata & Miller 1985);

degradation rate $k = 10^{-10} \text{ mol L}^{-1} \text{ d}^{-1}$ in freshwater and $k = 8^{-10} \text{ mol L}^{-1} \text{ d}^{-1}$ in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990).

Biotransformation: rate constant for bacterial transformation of $1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);

microbial transformation $k = (7.1 \pm 1.6) \times 10^{-11} \text{ L organism}^{-1} \text{ h}^{-1}$ (Paris et al. 1983; quoted, Steen 1991);

degradation $k = 3.49 \times 10^{-17} (\pm 38\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies (Banerjee et al. 1984).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: half-life in the atmosphere was estimated to be 1.96 d (Howard 1989); tropospheric lifetime of 1 d, calculated based on reactions principally with OH radical on March 21 at 43°N (Bunce 1991).

Surface water: $t_{1/2} = 16.8$ d in sludge and $t_{1/2} = 55.2$ d in polluted river waters (Mills et al. 1982); rate constant of $(1.1 \pm 0.3) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.8–4.0 (Hoigné & Bader 1983b); photolysis disappearance $k = 3.01 \times 10^{-2} \text{ min}^{-1}$ in the absence of DOM at 313 nm (Kawaguchi 1992).

Groundwater:

Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 14 d in Dunkirk silt loam, 47 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2} = 51$ d in a coarse sandy soil, $t_{1/2} = 110$ d in sandy loam (Kjeldsen et al. 1990)

$t_{1/2} = 7.2$ d in an acidic clay soil with < 1.0% organic matter and $t_{1/2} = 1.7$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota: $t_{1/2} < 1$ d in tissue of bluegill sunfish (Barrows et al. 1980).

TABLE 14.1.2.1.1

Reported aqueous solubilities and vapor pressures of 2-chlorophenol at various temperatures

Aqueous solubility				Vapor pressure	
Sidgwick & Turner 1922		Achard et al. 1996		Stull 1947	
synthetic method		shake flask-conductimetry		summary of literature data	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	P/Pa
−0.20	15600	15.4	24007	12.1	133.3
−0.30	24400	24.6	22660	38.2	666.6
82.9	37600	34.5	24007	51.2	1333
106.3	51200			65.9	2666
159.1	135800			82.0	5333
165.8	169500			92.0	7999
170.7	225900			106.0	13332
173.0	330000			126.4	26664
172.9	450400			149.8	53329
170.1	549500			174.5	101325
166.2	607200				
156.6	706200			mp/°C	7.0
118.9	828200				
91.5	859000				
−2.0	877300				
−4.0	892500				
−5.0	896200				
−8.0	908700				
−8.2	922000				
−6.0	929200				
−1.50	967900				
2.0	983900				
7.0	1000000				
critical solution temp 173°C					

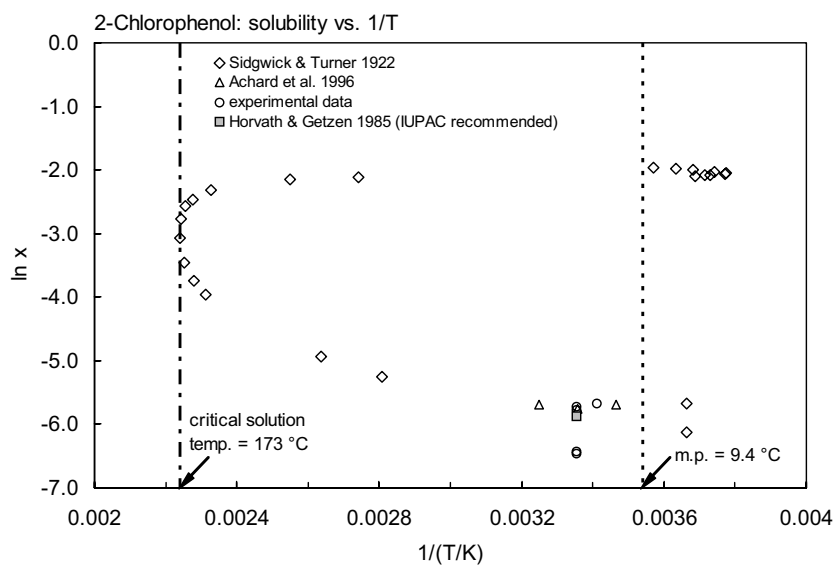


FIGURE 14.1.2.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-chlorophenol.

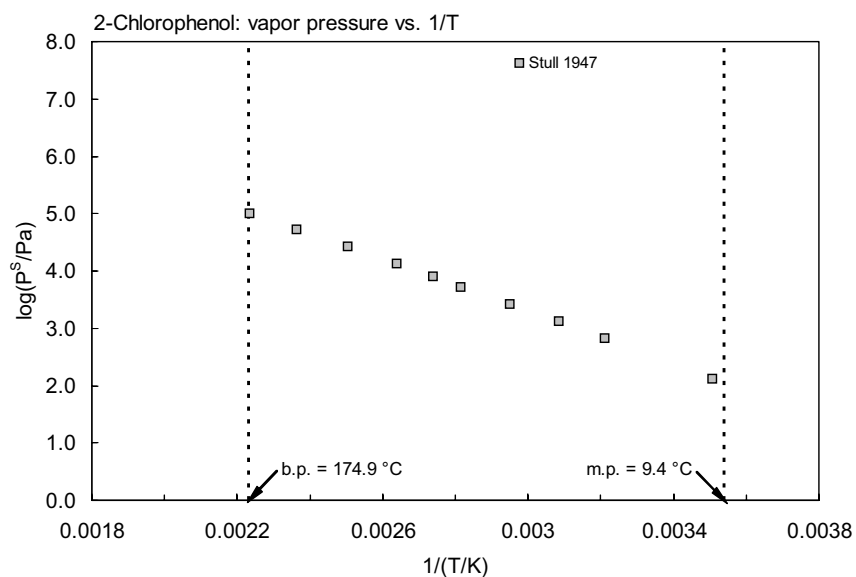
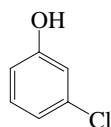


FIGURE 14.1.2.1.2 Logarithm of vapor pressure versus reciprocal temperature for 2-chlorophenol.

14.1.2.2 3-Chlorophenol



Common Name: 3-Chlorophenol

Synonym: *m*-chlorophenol, 1-chloro-3-hydroxybenzene

Chemical Name: 3-chlorophenol

CAS Registry No: 108-43-0

Molecular Formula: C₆H₄ClOH

Molecular Weight: 128.556

Melting Point (°C):

32.6 (Lide 2003)

Boiling Point (°C):

214.0 (Sidgwick & Turner 1922; Stull 1947; Weast 1982–83; Lide 2003)

Density (g/cm³, 20°C):

1.268 (25°C, Weast 1982–83)

Acid Dissociation Constant, pK_a:

9.12 (Farquharson et al. 1958; Renner 1990)

8.85 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)

9.08 (Pearce & Simkins 1968)

8.78 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988)

9.12 (Serjeant & Dempsey 1979; Howard 1989; Tratnyek & Hoigné 1991; Haderlein & Schwarzenbach 1993)

8.97 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Renner 1990; Ma et al. 1993)

9.10 (Dean 1985; Schultz & Cajina-Quezada 1987)

9.02 (Krijgsheld & van der Gen 1986)

9.37 (quoted from Ugland et al. 1981, Lagas 1988)

Molar Volume (cm³/mol):

103.3 (45°C, Stephenson & Malanowski 1987)

124.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

11.72 (Tsonopoulos & Prausnitz 1971)

14.91; 15.6 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

38.2 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol·K), F: 0.842 (mp at 9.4°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

26000* (20°C, synthetic method, measured range –0.20 to 130.8°C, Sidgwick & Turner 1922)

26000 (20–25°C, Seidell 1941; Urano et al. 1982; Shigeoka et al. 1988)

22420 (20°C, Mulley & Metcalf 1966)

22000 (recommended, Horvath & Getzen 1985)

22190 (shake flask-HPLC/UV at pH 4.6, Ma et al. 1993)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

41.90* (extrapolated-regression of tabulated data, temp range 44.2–214°C, Stull 1947)

41.40 (extrapolated-Antoine eq., liquid value, Weast 1972–73)

log (P/mmHg) = [–0.2185 × 11979.7/(T/K)] + 8.276287; temp range 44.2–214°C (Antoine eq., Weast 1972–73)

667.0 (72°C, Verschueren 1983)

1.034 (extrapolated-Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_s/\text{kPa}) = 7.61412 - 3178.132/(T/\text{K})$, temp range 252–293 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

33.40 (extrapolated-Antoine eq., supercooled liquid P_L , Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.54908 - 1978.86/(-51.572 + T/\text{K})$, temp range 317–487 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

0.0567 (calculated, Hine & Mookerjee 1975)

0.2045 (calculated-P/C, Shiu et al. 1994)

$k_H/\text{kPa} = 22.0921 - 6444.46/(T/\text{K})$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.50 (shake flask-UV, Fujita et al. 1964)

2.55 (calculated using data from Fujita et al. 1964, Umeyama et al. 1971)

2.52 (shake flask-UV, Korenman 1974)

2.17, 2.29 (calculated- π const., calculated-fragment const., Rekker 1977)

2.50 (Hansch & Leo 1979)

2.33 (HPLC- k' correlation, Butte et al. 1981, Butte et al. 1987)

2.44 (Dearden & Bresnen 1981)

2.36 (HPLC- k' correlation, Hammers et al. 1982)

2.55 (RP-HPLC- k' correlation, Miyake & Terada 1982)

1.87, 2.29 (HPLC- k' correlation, Eadsforth 1986)

2.36 (HPLC-RT correlation, Miyake et al. 1986)

2.55 (batch equilibration-UV, Beltrame et al. 1988)

2.50 (RP-HPLC-capacity ratio correlation, Minick et al. 1988)

2.48 (RP-HPLC, Shigeoka et al. 1988)

2.43; 2.63 (shake flask, HPLC-RT correlation, Wang et al. 1989)

2.50 (recommended, Sangster 1993)

2.64 (shake flask-GC, Kishino & Kobayashi 1994)

2.50; 2.57 (HPLC-RT correlation, electrometric titration, Slater et al. 1994)

2.50 (recommended, Hansch et al. 1995)

2.60 (solid-phase microextraction, Dean et al. 1996)

Bioconcentration Factor, $\log \text{BCF}$:

1.30 (Golden ide, Freitag et al. 1985)

1.25 (zebrafish, Butte et al. 1987)

0.845, 1.23 (earthworms *e. fetida andrei*: Kooyenberg soil, Holten soil, van Gestel & Ma 1988)

2.01, 2.09 (earthworms *I. rubellus*: Kooyenberg soil, Holten soil, van Gestel & Ma 1988)

1.17–2.55 (estimated from K_{ow} , Howard 1989)

1.00, 1.32, 2.17, 2.18 (earthworm system, from literature, Connell & Markwell 1990)

1.10, 1.40, 10.1, 16.3 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, $\log K_{oc}$:

1.20–2.74 (estimated from K_{ow} , Howard 1989)

2.54 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} \sim 73$ d for evaporation from a model river of 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: vapor phase $t_{1/2} = 1.96$ d (Howard 1989);

measured pseudo-first-order reaction $k = 0.048 \pm 0.001 \text{ min}^{-1}$ for direct photolysis in aqueous solutions (Peijnenburg et al. 1992).

Oxidation: rate constant $k = (5.4 \pm 1.0) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991).

Hydrolysis: will not be an important degradation process (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

completely degraded in soil suspensions within 72 d and by a soil microflora within 64 d (quoted, Verschuereen 1983);

time necessary for complete degradation of 16 mg/L in 14–25 d by wastewater (Haller 1978); degradation rate of $15 \text{ -mol L}^{-1} \text{ d}^{-1}$ in freshwater and $18 \text{ } \mu\text{mol L}^{-1} \text{ d}^{-1}$ in saline water with acclimated sulfidogenic sediment cultures (Hägglom & Young 1990).

Biotransformation: degradation rate of $4.32 \times 10^{-17} (\pm 47\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: vapor phase half-life was estimated to be 1.96 d (Howard 1989).

Surface water: $t_{1/2} = (14.5 \pm 0.3) \text{ min}$ for direct photolysis in aqueous solutions (Peijnenburg et al. 1992).

Ground water:

Sediment: half-life was approximately 30 d in sediment from a farm stream at 20°C (Howard 1989).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + d in Dunkirk silt loam, 47 + d in Mardin silt loam (Alexander & Aleem 1961)

disappearance $t_{1/2} = 2.5 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 5.4 \text{ d}$ from Holten soil with earthworms *e. fetida andrei* and $t_{1/2} = 2.6 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 2.1 \text{ d}$ from Holten soil with earthworms *I. rubellus* (van Gestel & Ma 1988);

$t_{1/2} = 15.1 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 21.8 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.2.2.1

Reported aqueous solubilities and vapor pressures of 3-chlorophenol at various temperatures

Aqueous solubility				Vapor pressure	
Sidgwick & Turner 1922				Stull 1947	
synthetic method				summary of literature data	
$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	P/Pa
−0.18	7300	3.2	844700	44.2	133.3
1.20	12500	−0.90	−*	72.0	666.6
2.5	18500	4.5	871900	86.1	1333
82.25	51200	−4.8	886600*	101.7	2666
118.0	111300	−8.2	901100*	118.0	5333
123.0	135600	−13.2	917300*	129.4	7999
127.5	178400	10.8	922300	143.0	13332
130.8	320200	−17.0	−*	164.8	26664
130.7	388900	17.0	951000	188.7	53329
130.5	461200	22.2	971100	214.0	101325
129.1	536500	32.5	1000000		
109.8	712300			mp/ $^\circ\text{C}$	32.5
23.1	823000	critical solution temp 130.8°C			
11.8	829000	*metastable point			

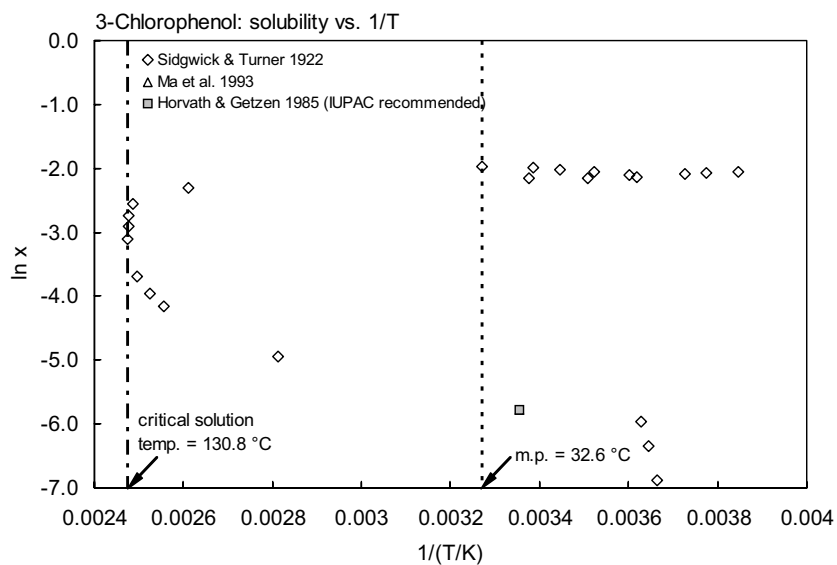


FIGURE 14.1.2.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-chlorophenol.

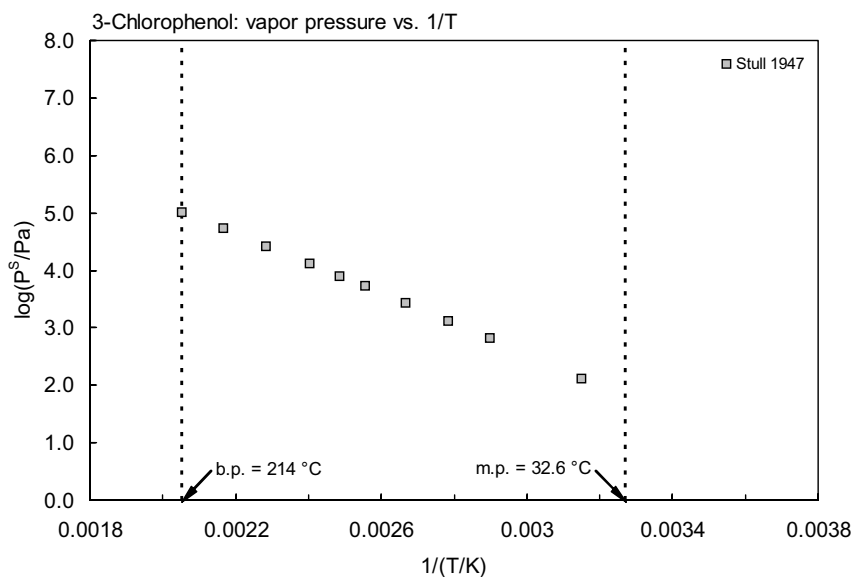
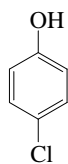


FIGURE 14.1.2.2.2 Logarithm of vapor pressure versus reciprocal temperature for 3-chlorophenol.

14.1.2.3 4-Chlorophenol



Common Name: 4-chlorophenol

Synonym: *p*-chlorophenol, 1-chloro-4-hydroxybenzene

Chemical Name: 4-chlorophenol

CAS Registry No: 106-48-9

Molecular Formula: $\text{ClC}_6\text{H}_4\text{OH}$

Molecular Weight: 128.556

Melting Point ($^{\circ}\text{C}$):

42.8 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

220 (Lide 2003)

Density (g/cm^3 at 20°C):

1.2651 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.37 (Farquharson et al. 1958; Ugland et al. 1981; Saarikoski & Viluksela 1982; Renner 1990)

9.18 (Doedens 1967)

9.42 (Pearce & Simkins 1968)

9.14 (Sillén & Martell 1971; Kaiser et al. 1984; Shigeoka et al. 1988; Argese et al. 1999)

9.41 (Serjeant & Dempsey 1979)

9.38 (Paris et al. 1982; Krijgsheld & van der Gen 1986)

9.20 (Hoigné & Bader 1983)

9.43 (Dean 1985; Schultz & Cajina-Quezada 1987)

9.37 ± 0.01 (potentiometric partition, Hersey et al. 1989)

9.57 ± 0.01 (UV with pH profile, Hersey et al. 1989)

Molar Volume (cm^3/mol):

101.6 (40°C , Stephenson & Malanowski 1987)

124.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

14.69 (Tsonopoulos & Prausnitz 1971)

14.07; 16.2 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

46.44 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, $F: 0.669$ (mp at 42.8°C))

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

27000* (20°C , synthetic method, measured range -0.20 to 128.7°C , Sidgwick & Turner 1922)

27000 (20 – 25°C , Seidell 1941; Urano et al. 1982)

27000 (shake flask-UV at pH 5.1, Blackman et al. 1955)

26250 (20°C , shake flask-UV, Mulley & Metcalf 1966)

24000 (shake flask-spectrophotometry, Roberts et al. 1977)

27000 (recommended, Horvath & Getzen 1985)

26390 (shake flask-HPLC/UV at pH 4.6, Ma et al. 1993)

25540* (25.2°C , shake flask-conductimetry, measured range 15.1 – 34.5°C , Achard et al. 1996)

20712* (11.05°C , shake flask-optical method, measured range 282.2 – 386.1 K , Jaoui et al. 1999)

25519* (24.85°C , shake flask-optical method, measured range 298 – 341.9 K , Jaoui et al. 2002)

$\ln [\text{S}/(\text{mol kg}^{-1})] = 5.6451 - 716.81/(\text{T}/\text{K})$; temp range 282 – 342 K (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 28.6* (extrapolated-regression of tabulated data, temp range 49.8–220°C, Stull 1947)
- 28.0 (extrapolated-Antoine eq., liquid value, Weast 1972–73)
- $\log(P/\text{mmHg}) = [-0.2185 \times 12281.6/(T/K)] + 8.331937$; temp range 49.8–220°C (Antoine eq., Weast 1972–73)
- 13.3, 33.3 (20°C, 30°C, Verschueren 1977, 1983)
- 3.47 (extrapolated liquid value, Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 8.83238 - 1385.1/(-131.1 + T/K)$, temp range 373–493 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C and reported temperature dependence equations):

- 0.0567 (calculated, Hine & Mookerjee 1975; Howard 1989)
- 0.0471 (calculated-P/C, Leuenberger et al. 1985)
- 0.0952 (calculated-P/C, Shiu et al. 1994)
- $k_H/\text{kPa} = 2017.07 - 110385.0/(T/K) - 290.078$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 2.39 (shake flask-UV, Fujita et al. 1964)
- 2.53 (shake flask-UV at pH 7.45, Umeyama et al. 1971)
- 2.37 (HPLC-RT correlation, Carlson et al. 1975)
- 2.40 (HPLC-RT correlation, Mirreles et al. 1976)
- 2.17, 2.29 (calculated- π const., calculated-fragment const., Rekker 1977)
- 2.35, 2.39, 2.44, 2.40 (lit. values, Hansch & Leo 1979)
- 2.51 (calculated- π const. or fragment const., McLeese et al. 1979)
- 2.55 (20°C, shake flask-UV, Rogers & Wong 1980)
- 2.35 (HPLC- k' correlation, Hammers et al. 1982)
- 2.51 (RP-HPLC- k' , correlation Miyake & Terada 1982)
- 2.46 ± 0.06 (HPLC-RV correlation.-ALPM, Garst & Wilson 1984)
- 2.88 (CPC-RV, Terada et al. 1987)
- 2.43 (batch equilibration-UV, Beltrame et al. 1988, Beltrame et al. 1989)
- 2.39 (RP-HPLC-capacity ratio, Minick et al. 1988)
- 2.41 (shake flask, Shigeoka et al. 1988)
- 2.42; 2.46; 2.34, 2.45 (filter chamber-UV; potentiometric partition; Hersey et al. 1989)
- 2.52; 2.59 (shake flask; HPLC-RT correlation, Wang et al. 1989)
- 2.39 (recommended, Sangster 1993)
- 2.63 (shake flask-GC, Kishino & Kobayashi 1994)
- 2.41; 2.45 (HPLC-RT correlation, electrometric titration, Slater et al. 1994)
- 2.39 (recommended, Hansch et al. 1995)
- 1.82, 1.83, 2.01, 1.98 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, $\log BCF$:

- 1.18 (goldfish, Kobayashi et al. 1979)
- 0.30–1.59 (estimated from K_{OW} , Howard 1989)
- 1.05–1.50 (estimated, NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 1.85 (clay loam soil, Boyd 1982; Howard 1989)
- 1.20–2.68 (estimated from K_{OW} , Howard 1989)
- 2.377, 2.686, 2.025, 2.222, 2.332 (soils, first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998)
- 2.142, 1.966, 1.966, 2.289, 1.952 (soils, second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: half-lives of 12.8 h, 17.4 h for evaporation from stirred and static water at a depth of 0.38 cm at 23.6°C (Chiou et al. 1980; Howard 1989); $t_{1/2} = 73$ d was estimated for evaporation from a river 1 m deep, flowing at 1 m/s with a wind velocity of 3 m/s (Howard 1989).

Photolysis:

photo-transformation rate constants: $k = 0.011 \text{ h}^{-1}$ with $t_{1/2} = 63$ h for distilled water in summer (mean temp 25°C) and $k = 0.007 \text{ h}^{-1}$ with $t_{1/2} = 99$ h in winter (mean temp 14°C); $k = 0.03 \text{ h}^{-1}$ with $t_{1/2} = 28$ h for estuarine water in summer and $k = 0.011 \text{ h}^{-1}$ with $t_{1/2} = 63$ h in winter exposed to full sunlight and microbes (Hwang et al. 1986)

photo-mineralization rate constants: $k = 0.012 \text{ h}^{-1}$ with $t_{1/2} = 58$ d for distilled water in summer and $k = 0.003 \text{ h}^{-1}$ with $t_{1/2} = 224$ d in winter; $k = 0.07 \text{ h}^{-1}$ with $t_{1/2} = 10$ d in summer and $k = 0.007 \text{ h}^{-1}$ with $t_{1/2} = 95$ d in winter for surface estuarine water exposed to full sunlight and microbes (Hwang et al. 1986);

photo-degradation $k = 564 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 1.1$ min for direct UV radiation in aqueous solutions (Benitez et al. 2000).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(\text{aq.}) = (600 \pm 100) \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone in water using 1 mM PrOH as scavenger at pH 2 and 20–23°C (Hoigné & Bader 1983a)

$k(\text{aq.}) = 34 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, and $k = (600 \pm 100) \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k = (0.6 \pm 0.2) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.5–6 and 20–23°C (Hoigné & Bader 1983b)

$k(\text{aq.}) = (6.0 \pm 3.6) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991)

72.1 mg/L total organic carbon (TOC) degraded to 98% TOC after 5 h illumination with 250 watt tungsten lamp by the photo-Fenton reaction (Ruppert et al. 1993)

$k = 1877 \times 10^3 \text{ min}^{-1}$ with a half-life of 0.4 min for reaction with Fenton's reagent; $k_{\text{O}_3} = 17 \times 10^3 \text{ min}^{-1}$ with a half-life of 38.15 min at pH 2; and $k_{\text{O}_3} = 239 \times 10^3 \text{ min}^{-1}$ with a half-life of 3.4 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000)

Hydrolysis:

Biodegradation: 95% degradation in 3–6 d in a mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $11.0 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mg/L in 7–14 d by wastewater and in 14–25 d by soil (Haller 1978);

$t_{1/2} = 475$ h in river waters with a calculated first-order $k = 0.035 \text{ d}^{-1}$ (Lee & Ryan 1979; quoted, Battersby 1990);

aerobic degradation in a non-sterile clay-loam soil: 77% loss at 0°C at the termination of the experiment after 14 d, 84% loss at 4°C after 12 d and 100% loss at 20°C after 30 d all under same experimental conditions (Baker et al. 1980);

$t_{1/2} = 216$ –480 h and 72–1080 h for 75% degradation in mineral medium and seawater (de Kreuk & Hanstveit 1981);

biodegradation first order rate constant $k = 0.23 \text{ d}^{-1}$ in aquatic systems (Scow 1982);

completely degraded in soil suspensions in 9 d and by a soil microflora in 16 d (quoted, Verschueren 1983);

microbial degradation is the primary transformation process; transformation $k = 0.06 \text{ h}^{-1}$ with $t_{1/2} = 11$ h for estuarine water in summer and $t_{1/2} = 0.006 \text{ h}^{-1}$ with $t_{1/2} = 116$ h in winter in the darkness (Hwang et al. 1986)

mineralization $k = 0.293 \text{ h}^{-1}$ with $t_{1/2} = 2$ d for estuarine water in summer and $k = 0.003 \text{ h}^{-1}$ with $t_{1/2} = 231$ d in winter in the darkness (Hwang et al. 1986); degradation rate constants $k = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 480$ d in Skidway River water and 0.23 d^{-1} with a half-life of 72 h in Skidway River water-sediment slurry (Pritchard 1987); degradation rate constant of $37 \mu\text{mol L}^{-1} \text{ d}^{-1}$ in freshwater and $22 \mu\text{mol L}^{-1} \text{ d}^{-1}$ in saline water with acclimated sulfidogenic sediment cultures (Häggblom & Young 1990);

average transformation rate of $53 \mu\text{mol L}^{-1} \text{ d}^{-1}$ at 31°C for anaerobic degradation in freshwater sediments with an average adaptation time of 37 d (Zhang & Wiegel 1990);

70% degradation within 1–2 d in soil and completely degraded within 15 d in river water (NCASI 1992)

Degradation constant $k = 8.5 \mu\text{M/h}$ for aerobic dechlorination in shake flask experiments;; $k = 10 \mu\text{M/h}$ in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999).

Biotransformation: microbial transformation rate constant of $(1.7 \pm 0.9) \times 10^{-12}$ L organism⁻¹ h⁻¹ (Paris et al. 1982); microbial transformation rate constant of $(4.7 \pm 1.6 \times 10^{-11}$ L organism⁻¹ h⁻¹ to $(9.0 \pm 1.7) \times 10^{-11}$ L organism⁻¹ h⁻¹ in pond and river samples at five different sites (Paris et al. 1983); degradation rate $k = 5.44 \times 10^{-17}$ ($\pm 32\%$ SD) mol cell⁻¹ h⁻¹ from pure culture studies and 0.3×10^{-12} mol cell⁻¹ h⁻¹ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 1.96$ d in the atmosphere (Howard 1989)

Surface water: $t_{1/2} = 475$ h for biodegradation in river waters with a calculated first-order rate constant of 0.035 d⁻¹ (Lee & Ryan 1979; quoted, Battersby 1990);

$t_{1/2} = 216$ –624 h and 72–1080 h for 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hanstveit 1981);

rate constant $k = 600 \pm 100$ M⁻¹ s⁻¹ for the reaction with ozone at pH 1.5–6.0 (Hoigné & Bader 1983);

$t_{1/2} = 63$ h in summer at season temp., 25°C, $t_{1/2} = 99$ h in winter at season temp., 14°C in distilled water and 28 h in summer, $t_{1/2} = 63$ h in winter in estuary surface water, based on photo-transformation rate (Hwang et al. 1986);

$t_{1/2} = 58$ d in summer, $t_{1/2} = 224$ d in winter in distilled water; and $t_{1/2} = 10$ d in summer, $t_{1/2} = 95$ d in winter in surface estuarine water, based on photo-mineralization rate (Hwang et al. 1986);

$t_{1/2} = 216$ h at 21°C in Skidway River water (Pritchard 1987);

$t_{1/2} = 20$ d in water (Howard 1989);

at a concentration of 1 mg/L, 4-CP was degraded completely within 15 d in river waters (NCASI 1992);

photo-oxidation $t_{1/2} = 0.4$ min for reaction with Fenton's reagent; $t_{1/2} = 38.15$ min at pH 2, and $t_{1/2} = 3.4$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water:

Sediment: $t_{1/2} = 72$ h at 22°C in Skidway River water-sediment slurry (Pritchard 1987);

$t_{1/2} = 3$ d in sediment and seawater (Howard 1989).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 9 d in Dunkirk silt loam, 3 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2} = 2.5$ d in an acidic clay soil with < 1.0% organic matter and $t_{1/2} = 1.0$ d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992);

70% degradation with 1 to 2 d (NCASI 1992).

Biota:

TABLE 14.1.2.3.1

Reported aqueous solubilities of 4-chlorophenol at various temperatures

Sidgwick & Turner 1922		Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002	
synthetic method		shake flask-conductivity		shake flask-optical method		shake flask-optical method*	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³
–0.20	20700	15.1	23337	282.2	17856.	298.0	25519
65.0	39100	25.2	25540	284.2	20712	305.2	27010
113.8	106600	34.6	28499	308.3	27855	315.3	29389
125.0	205000			311.2	29283	319.7	30057
128.2	291600			324.2	32140	323.8	30919
128.7	425700			341.9	35711	332.7	32809
125.8	534900			354.7	41425	341.2	34608
122.4	596200			359.9	44282	298.0	25519
115.5	650500			362.7	48567	305.2	27010
107.7	693600			364.4	52852	315.3	29132
97.0	740300			365.7	54261	332.7	32809

(Continued)

TABLE 14.1.2.3.1 (Continued)

Sidgwick & Turner 1922		Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002	
synthetic method		shake flask-conductivity		shake flask-optical method		shake flask-optical method*	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³
35.5	840200			366.7	57852	339.5	34248
17.0	854200			386.1	117132	298.3	25583
5.5	861900					309.3	27872
0.5	889200					315.8	29235
6.2	924800					324.8	31124
11.0	944800					329.0	32024
14.2	957000					341.9	34763
18.0	968200						
19.5	972900						
41.0	1000000						
critical solution temp 129°C							
triple point -0.30°							

*some data from Achard et al.
1996, Jaoui et al. 1999

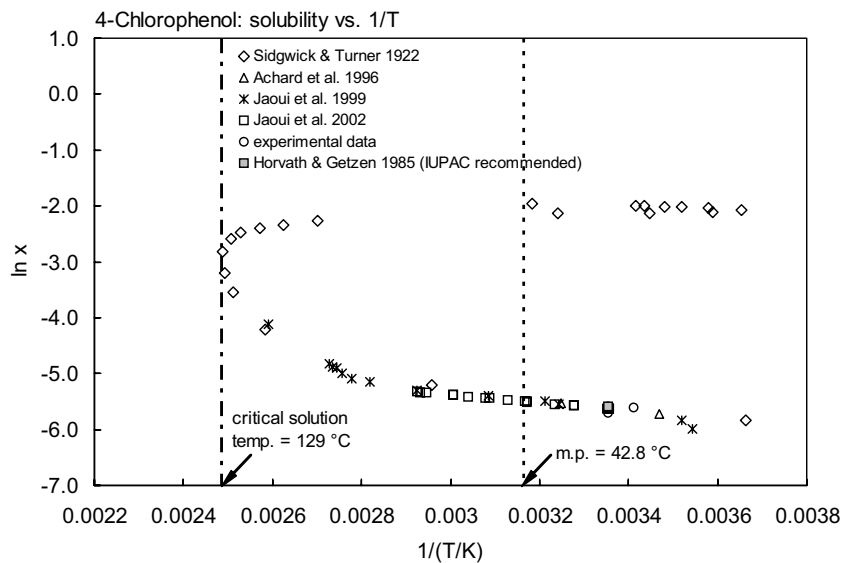


FIGURE 14.1.2.3.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-chlorophenol.

TABLE 14.1.2.3.2
Reported vapor pressures of 4-chlorophenol at various temperatures

Stull 1947
 summary of literature data

t/°C	P/Pa
49.8	133.3
78.2	666.6
92.2	1333
108.1	2666
125.0	5333
136.1	7999
150.0	13332
172.0	26664
196.0	53329
220.0	101325
mp/°C	42.0

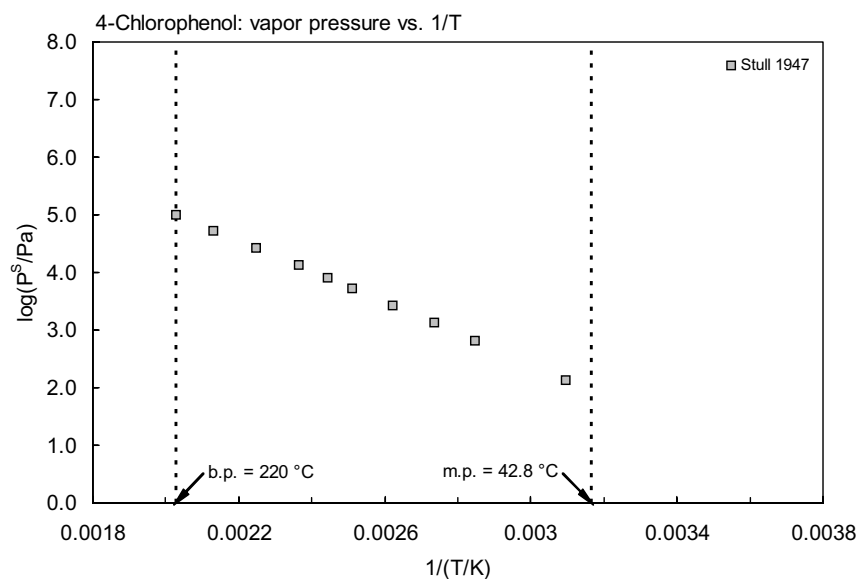
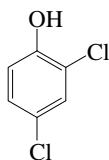


FIGURE 14.1.2.3.2 Logarithm of vapor pressure versus reciprocal temperature for 4-chlorophenol.

14.1.2.4 2,4-Dichlorophenol



Common Name: 2,4-Dichlorophenol

Synonym: 2,4-DCP

Chemical Name: 2,4-dichlorophenol

CAS Registry No: 120-83-2

Molecular Formula: $C_6H_4Cl_2O$, $C_6H_3Cl_2OH$

Molecular Weight: 163.001

Melting Point ($^{\circ}C$):

45.0 (Stull 1947; Verschueren 1977, 1983; Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

210.0 (Stull 1947; Verschueren 1977, 1983; Weast 1982–83; Lide 2003)

Density (g/cm^3):1.383 (at 60/ $25^{\circ}C$, Verschueren 1983)Acid Dissociation Constant, pK_a :

7.80 (Blackman et al. 1955; Hoigné & Bader 1983; Scully & Hoigné 1987)

7.85 (Farquharson et al. 1958; Pearce & Simkins 1968)

7.68 (Doedens 1967)

7.89 (Sillén & Martell 1971; Serjeant & Dempsey)

8.01, 8.04, 8.09 (measured values, Xie & Dyrssen 1984)

8.09 (Shigeoka et al. 1988)

Molar Volume (cm^3/mol):

145.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.09; 16.7 (exptl.; calculated-group additivity method, Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.636 (mp at $45^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4500 (gravimetric, Mosso 1887)

6194 (shake flask-UV at pH 5.1, Blackman et al. 1955)

5000 (shake flask-spectrophotometry, Roberts et al. 1977)

2650 (shake flask-GC, Jones et al. 1977/1978)

4600 ($20^{\circ}C$, Verschueren 1977, 1983)

5547 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)

4600 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

5517* ($25.2^{\circ}C$, shake flask-conductimetry, measured range 15.3 – $35.1^{\circ}C$, Achard et al. 1996)6339* ($37.35^{\circ}C$, shake flask-optical method, measured range 310.5 – $423.2 K$, Jaoui et al. 1999)

4980 (shake flask-HPLC/UV, pH 4.98, Huang et al. 2000)

4841* ($21.45^{\circ}C$, shake flask-optical method, measured range 296.4 – $337.7 K$, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 11.846 - 3025.1/(T/K)$; temp range 288 – $298 K$ (eq.-I derived using reported exptl. data, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 5.0497 - 981.37/(T/K)$; temp range 298 – $347 K$ (eq.-II derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 20.6* (extrapolated-regression of tabulated data, temp range 53–210°C, Stull 1947)
- 11.9 (extrapolated-Antoine eq., Weast 1972–73)
- $\log(P/\text{mmHg}) = [-0.2185 \times 13230.4/(T/K)] + 8.884810$; temp range 53–210°C (Antoine eq., Weast 1972–73)
- 18.0 (supercooled liquid value, GC-RT correlation, Hamilton 1980)
- 15.4 (capillary GC-RT, Bidleman & Renberg 1985)
- 2.40, 11.87 (8°C, 25°C, extrapolated, Leuenberger et al. 1985)
- $\log(P_L/\text{kPa}) = 6.75941 - 1945.1/(-73.987 + T/K)$; temp range 326–483 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 6.32554 - 1807.32/(-69.17 + T/K)$; temp range 391–474 K (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 0.284 (calculated-P/C, Mabey et al. 1982)
- 0.110 (8°C, calculated-P/C, Leuenberger et al. 1985)
- 0.435 (calculated-P/C, Shiu et al. 1994)
- $k_H/\text{kPa} = 24.9070 - 6791.07/(T/K)$; temp range 323–363 K (activity coefficient by ebulliometric method, Tabai et al. 1997)
- 0.292 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.08 (Leo et al. 1971)
- 3.06 (shake flask-UV, Stockdale & Selwyn 1971)
- 3.06, 3.08 (Hansch & Leo 1979)
- 2.92 (HPLC- k' correlation, Hammers et al. 1982)
- 3.14 (RP-HPLC- k' correlation, Miyake & Terada 1982)
- 3.41 (shake flask-UV, Beltrame et al. 1984)
- 3.23 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 3.20, 3.17, 3.17 (20°C, shake flask-GC-calculated-regression, Xie & Dyrssen 1984)
- 3.21, 3.23 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
- 3.23 (OECD 1981 guidelines, Leuenberger et al. 1985)
- 2.87 (RP-HPLC-RT correlation, Chin et al. 1986)
- 2.97 (HPLC-RT correlation, Miyake et al. 1986)
- 3.61 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
- 3.21 (shake flask, Shigeoka et al. 1988; quoted, Saito et al. 1993)
- 3.16 (shake flask/batch equilibrium-UV, Beltrame et al. 1988)
- 3.06 (EPA CLOGP Data Base, Hulzebos et al. 1993)
- 3.17 (recommended, Sangster 1993)
- 3.07 (calculated-QSAR, Kollig 1993)
- 3.20 (shake flask-GC, Kishino & Kobayashi 1994)
- 3.06 (recommended, Hansch et al. 1995)
- 3.34 (solid-phase microextraction; Dean et al. 1996)

Bioconcentration Factor, $\log BCF$:

- 1.53 (goldfish, Kobayashi 1979)
- 1.00 (trout, Hattula et al. 1981)
- 2.27 (microorganism-water, calculated- K_{OW} , Mabey et al. 1982)
- 2.00 (golden ide, after 3 d, Freitag et al. 1985)
- 2.42 (algae, after 1 d, Freitag et al. 1985)
- 2.53 (activated sludge, after 5 d, Freitag et al. 1985)
- 1.00 (quoted, brown trout, Walden et al. 1986)
- 1.80 (correlated, Isnard & Lambert 1988)
- 1.41–1.65 (estimated, NCASI 1992)

Sorption Partition Coefficient, log K_{OC} :

- 2.59 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 2.59–3.02 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 2.89–3.12 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 2.10–2.32 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 2.48–2.91 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 1.74–2.13 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 3.60, 3.50 (untreated fine and coarse sediment, Isaacson & Frink 1984)
 3.71, 3.98 (treated fine and coarse sediment, Isaacson & Frink 1984)
 2.75 (sediment, Schenllenberg et al. 1984; quoted, Sabljic 1987a,b)
 2.76 (soil, calculated-MCI χ , Sabljic 1987a,b)
 2.49 (calculated- K_{OW} , Kollig 1993)
 2.75 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.47, 2.53 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 2.609, 2.654, 2.460, 2.346, 2.540 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)
 2.49, 2.57, 2.77, 2.33 (soils: organic carbon OC -0.1% and pH 2.0–7.4, OC -0.1% and pH ≤ 5.8 , OC -0.5%, $0.1 \leq OC < 0.5\%$, average, Delle Site 2001)

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

photolysis:

$k_p = 0.82 \text{ h}^{-1}$ with $t_{1/2} = 0.8 \text{ h}$ for distilled water in summer at mean temp. 25°C , and $k_p = 0.21 \text{ h}^{-1}$ with $t_{1/2} = 3 \text{ h}$ in winter at mean temp. 11°C ; $k_p = 1.16 \text{ h}^{-1}$ with $t_{1/2} = 0.6 \text{ h}$ for estuarine water in summer and $k_p = 0.44 \text{ h}^{-1}$ with $t_{1/2} = 2 \text{ h}$ in winter; $k_p = 1.0 \text{ h}^{-1}$ with $t_{1/2} = 0.7 \text{ h}$ in summer and $k_p = 0.38 \text{ h}^{-1}$ with $t_{1/2} = 2 \text{ h}$ in winter for poisoned estuarine water when exposed to full sunlight and microbes (photo-transformation, Hwang et al. 1986)

$k_p = 0.09 \text{ h}^{-1}$ with $t_{1/2} = 8 \text{ d}$ in summer and $k_p = 0.049 \text{ h}^{-1}$ with $t_{1/2} = 14 \text{ d}$ in winter for distilled water; $k_p = 0.20 \text{ h}^{-1}$ with $t_{1/2} = 4 \text{ d}$ in summer and $k_p = 0.04 \text{ h}^{-1}$ with $t_{1/2} = 17 \text{ d}$ in winter for estuarine water; $k_p = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ in summer and $k_p = 0.05 \text{ h}^{-1}$ with $t_{1/2} = 14 \text{ d}$ in winter for poisoned estuarine water when exposed to full sunlight and microbes (photo-mineralization rate, Hwang et al. 1986)

photochemical-transformation $t_{1/2} = 2.5\text{--}2.6 \text{ h}$ in Xenotest 1200 (Svenson & Björndal 1988)

atmospheric and aqueous photolysis $t_{1/2} = 0.8\text{--}3 \text{ h}$ based on measured rate of photolysis in distilled water under sunlight in summer and winter (Howard et al. 1991)

$k_p = 38 \times 10^3 \text{ min}^{-1}$ with a $t_{1/2} = 17.5 \text{ min}$ for direct UV radiation aqueous solutions (Benitez et al. 2000)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k < 7 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen, and $1 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982)

$k = 5 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, $k < 1.5 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k = (8 \pm 4) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.3–1.5 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983b)

$k = 7 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.5, $k = 2 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 6.0, $k = 10 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 6.6, $k = 15 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.0, $k = 76 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7.9, $k = 120 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9.0 and pH 9.6 for the reaction with singlet oxygen in water at $19 \pm 2^\circ\text{C}$ (Scully & Hoigné 1987)

$k_{OH} = 1.06 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson 1989)

$k_{OH} = 3.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Bunce et al. 1991)

$k = (5.1 \pm 4.7) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991)

$k_{OH}(\text{calc}) = 1.71 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital estimation method, Klamt 1993)

$k = 209 \times 10^3 \text{ min}^{-1}$ with a half-life of 2.4 min for reaction with Fenton's reagent; and $k = 24 \times 10^3 \text{ min}^{-1}$ with a half-life of 30.4 min at pH 2, and $k = 315 \times 10^3 \text{ min}^{-1}$ with a half-life of 3.3 min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000)

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: 7 to 10 d for bacteria to utilize 95% of 200 ppm in parent substrate (Tabak et al. 1964);

aqueous aerobic $t_{1/2} = 66.7\text{--}199$ h, based on aerobic lake die-away test data (Aly & Faust 1964; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 324\text{--}1032$ h, based on anaerobic lake die-away test data (Aly & Faust 1964; selected, Howard et al. 1991);

completely degraded in soil suspensions in 9 d (Woodcock 1971; quoted, Verschueren 1983);

average rate of biodegradation $10.5 \text{ mg COD g}^{-1} \text{ h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20-d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

aerobic degradation in a non-sterile clay-loam soil: 79% loss at 0°C at the termination of the experiment after 14 days, 82% loss at 4°C after 12 d and 84% loss at 20°C after 40 d all under same experimental conditions (Baker et al. 1980);

rate constants $k = 0.5 \text{ d}^{-1}$ with $t_{1/2} = 1.4$ d in adapted activated sludge and $k = 0.1 \text{ d}^{-1}$ with $t_{1/2} = 6$ d in natural waters under anaerobic conditions (Mills et al. 1982);

microbial degradation negligible in darkness (Hwang et al. 1986);

$k = 0.223 \text{ h}^{-1}$ for maximum removal by activated sludge microorganisms (Chudoba et al. 1989);

biodegradation first-order rate of hydroxylation, $k = 0.017 \text{ min}^{-1}$ by *pseudomonas putida* Fl (Spain et al. 1989; quoted, Neilson et al. 1991);

15% reduction in concn ($2 \mu\text{M}$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

transformation rate of $245 \text{ -mol L}^{-1} \text{ d}^{-1}$ at 31°C for anaerobic degradation in freshwater sediments with an average of 7 d adaptation time (Zhang & Wiegel 1990);

complete biodegradation in water, seawater, sludge and lagoon within 16 to 23 d (NCASI 1992).

Degradation constant $k = 1.6 \mu\text{M/h}$ for anaerobic batch experiment in serum bottles; $k = 1.2 \mu\text{M/h}$ for dechlorination in anaerobic batch or continuous bioreactor; $k = 1.9 \mu\text{M/h}$ in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999)

Biotransformation: for bacterial transformation $k = 1 \times 10^7 \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);

degradation rate $k = 3.76 \times 10^{-19} \text{ mol cell}^{-1} \text{ h}^{-1}$ ($\pm 47\%$ SD) from pure culture studies, $k = 0.02 \times 10^{-14}$ to $2 \times 10^{-14} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated tropospheric lifetime of 3 d for reaction with OH radical on March 21 at 43°N ; lifetime varies from 2 to 20 d at the latitude of Toronto depending on seasons; at latitude of 43.7°N , tropospheric lifetimes are: 20 d on December 21, 5 d on February 21, 2.2 d on April 21 and 1.5 d on June 21; and at different geographical locations on March 21, lifetimes are 1.7 d at latitude 0° , 2.2 d at 25°S , 6.7 d at 55°S and 680 at 85°S (Bunce et al. 1991);

$t_{1/2} = 21.2\text{--}212$ h, based on estimated rate constant for reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: rate constant $k < 1.5 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 1.5–3.0 (Hoigné & Bader 1983);

$t_{1/2} = 0.8$ h in summer, $t_{1/2} = 3.0$ h in winter for distilled water; $t_{1/2} = 0.7$ h in summer, $t_{1/2} = 2.0$ h in winter for poisoned estuarine water; $t_{1/2} = 0.6$ h in summer, $t_{1/2} = 2.0$ h in winter for estuarine water, all based on photo-transformation rate under full sunlight and microbes; $t_{1/2} = 8.0$ d in summer, $t_{1/2} = 14$ d in winter for distilled water; $t_{1/2} = 6$ d in summer, $t_{1/2} = 14$ d in winter for poisoned estuarine water and $t_{1/2} = 4$ d in summer, $t_{1/2} = 17$ d in winter for estuarine water, based on photo-mineralization rate under full sunlight and microbes (Hwang et al. 1986);

$t_{1/2} = 62$ h in water at pH 8 and $19 \pm 2^\circ\text{C}$ for the reaction with singlet oxygen (Scully & Hoigné 1987);

$t_{1/2} = 2.5\text{--}2.6$ h for photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2} = 0.8\text{--}3$ h based on measured rate of photolysis in distilled water under sunlight in summer and winter (Howard et al. 1991);

complete biodegradation within 5–23 d in seawater (NCASI 1992);

photo-oxidation $t_{1/2} = 2.4$ min for reaction with Fenton's reagent; $t_{1/2} = 30.4$ min at pH 2 and $t_{1/2} = 3.3$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{1/2} = 133\text{--}1032$ h, based on unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: mean half-life of dechlorination: $t_{1/2} = 116$ d in July and $t_{1/2} = 47$ d in November (Hale et al. 1991).

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 9 d in Dunkirk silt loam, 3 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2} = 176\text{--}1680$ h, based on aerobic soil die-away test data (Baker et al. 1980; Haider et al. 1974; selected, Howard et al. 1991);

$t_{1/2} = 3.5$ d in an acidic clay soil with $< 1.0\%$ organic matter and 1.5 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.2.4.1

Reported aqueous solubilities and vapor pressures of 2,4-dichlorophenol at various temperatures

Aqueous solubility						Vapor pressure	
Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002		Stull 1947	
shake flask-conductivity		shake flask-optical method		shake flask-optical method*		summary of literature data	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³	t/°C	P/Pa
15.3	3896	310.5	6339	294.6	4841	53.0	133.3
25.2	5517	327.1	7244	303.1	6129	80.0	666.6
29.8	6075	338.1	8150	311.5	6683	92.8	1333
35.1	6501	347.2	9056	322.4	7433	107.7	2666
		355.1	9961	336.7	8460	123.4	5333
		363.5	10867	295.2	4939	133.5	7999
		373.7	10867	303.7	6161	146.0	13332
		382.1	11772	312.4	6748	165.2	26664
		393.5	12678	318.1	7139	187.5	53329
		401.5	13583	232.2	7482	210.0	101325
		408.4	14489	291.4	4320		
		423.2	15394	302.0	6047	mp/°C	45.0
				308.8	6504		
				321.0	7335		
				337.7	8525		

*some data from Achard et al.
1996, Jaoui et al. 1999

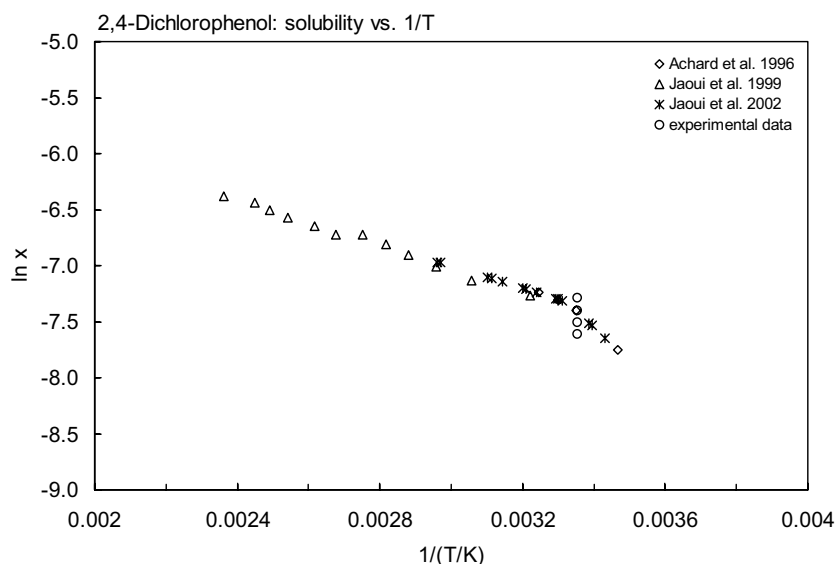


FIGURE 14.1.2.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,4-dichlorophenol.

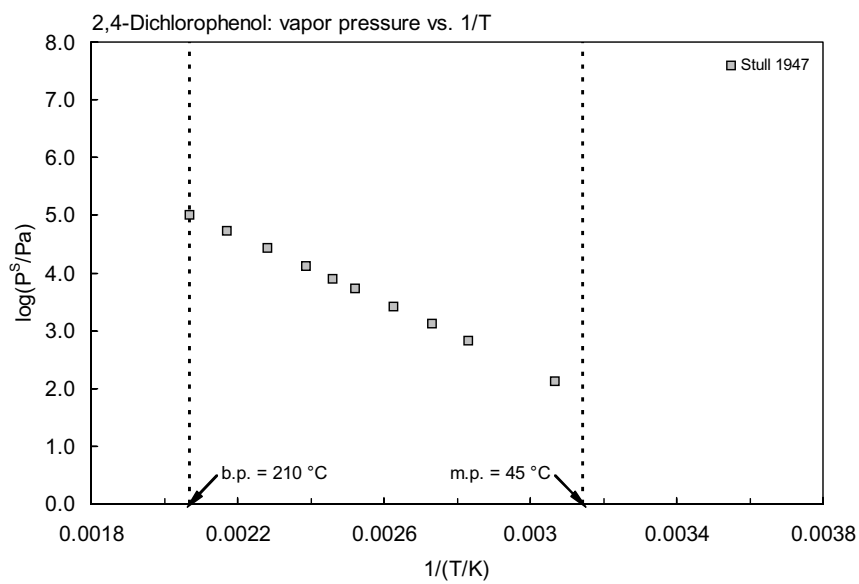
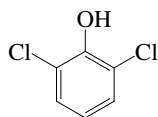


FIGURE 14.1.2.4.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4-dichlorophenol.

14.1.2.5 2,6-Dichlorophenol



Common Name: 2,6-Dichlorophenol

Synonym: 2,6-DCP

Chemical Name: 2,6-dichlorophenol

CAS Registry No: 87-65-0

Molecular Formula: $C_6H_3Cl_2OH$

Molecular Weight: 163.001

Melting Point ($^{\circ}C$):

68.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

220 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.91 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

6.80 (Doedens 1967; McLeese et al. 1979)

6.79 (Pearce & Simkins 1968)

6.79 (Sillén & Martell 1971; Kaiser et al. 1984; Xie & Dyrssen 1984; Shigeoka et al. 1988)

6.78 (Ugland et al. 1981; Dean 1985)

6.54 (Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

145.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

22.14 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$, F: 0.374 (mp at $68.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2625 (shake flask-HPLC/UV at pH 4.5, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13.1* (extrapolated-regression of tabulated data, temp range 59.5 – $220^{\circ}C$, Stull 1947)

12.9 (extrapolated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 13472.0/(T/K)] + 8.864007$; temp range 59.5 – $220^{\circ}C$ (Antoine eq., Weast 1972–73)

12.2 (supercooled liq. value, GC-RT correlation, Hamilton 1980)

12.7 (capillary GC-RT, Bidleman & Renberg 1985)

11.2 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.32845 - 2436.59/(-35.584 + T/K)$; temp range 333 – $493\ K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 5.2254 - 1106.4/(-151.42 + T/K)$; temp range 353 – $493\ K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.7376 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.86 (Hansch & Leo 1979)

2.34 (HPLC-RT correlation, Butte et al. 1981)

2.64 (HPLC- k' correlation, Hammers et al. 1982)

3.36	(shake flask-UV, Beltrame et al. 1984)
2.84, 2.92	(shake flask-GC, HPLC-k' correlation, Xie et al. 1984)
2.84	(shake flask, Shigeoka et al. 1988)
2.80	(batch equilibration-UV, Beltrame et al. 1988)
2.64	(recommended, Sangster 1993)
2.92	(shake flask-GC, Kishino & Kobayashi 1994)
2.75	(recommended, Hansch et al. 1995)
2.57	(HPLC-RT correlation, Makovskaya et al. 1995b)

Bioconcentration Factor, log BCF:

1.44–1.56 (estimated, NCASI 1992)

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

Photolysis:

Photooxidation:

Hydrolysis:

Biodegradation: 1920 - ∞ h and 144–360 h for 75% degradation in mineral medium and seawater batch experiments respectively (de Kreuk & Hanstveit 1981)

81% reduction in concn (2 μ M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2}$ = 1920 - ∞ h and 144–360 h for 75% degradation in mineral medium and seawater batch experiments, respectively (de Kreuk & Hanstveit 1981).

Ground water:

Sediment:

Soil: $t_{1/2}$ = 16.2 d in an acidic clay soil with < 1.0% organic matter and $t_{1/2}$ = 2.4 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).

Biota:

TABLE 14.1.2.5.1
Reported vapor pressures of 2,6-dichlorophenol at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
59.5	133.3
87.5	666.6
101.0	1333
115.5	2666
131.5	5333
141.8	7999
154.6	13332
175.5	26664
197.7	53329
220.0	101325
mp/°C	-

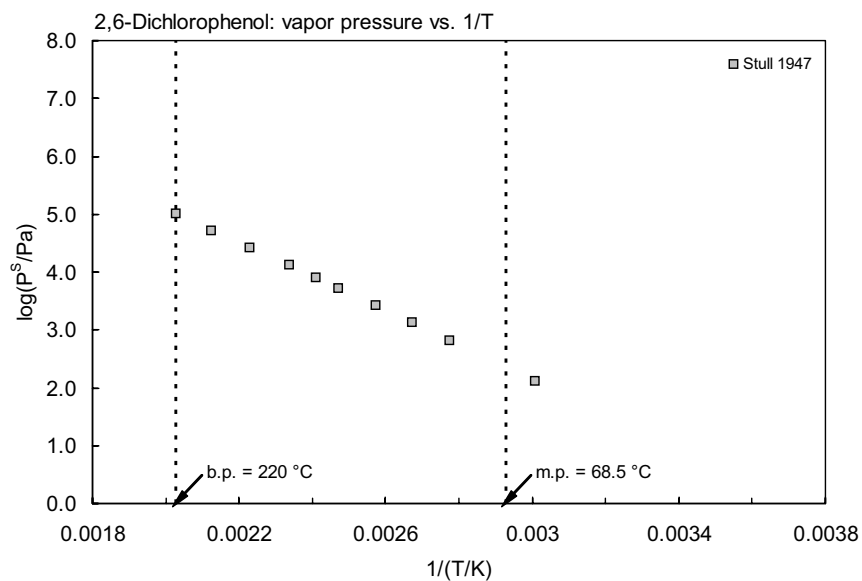
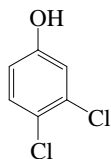


FIGURE 14.1.2.5.1 Logarithm of vapor pressure versus reciprocal temperature for 2,6-dichlorophenol.

14.1.2.6 3,4-Dichlorophenol



Common Name: 3,4-Dichlorophenol

Synonym: 3,4-DCP

Chemical Name: 3,4-dichlorophenol

CAS Registry No: 95-77-2

Molecular Formula: $C_6H_3Cl_2OH$

Molecular Weight: 163.001

Melting Point ($^{\circ}C$):

68.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

253 (Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.39 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)

8.59 (Pearce & Simkins 1968; Serjeant & Dempsey 1979; Hammers et al. 1982)

8.59 (Sillén & Martell 1971; Kaiser et al. 1984)

8.62 (Ugland et al. 1981; Lagas 1988; Renner 1990; Ma et al. 1993)

8.68 (Xie & Dyrssen 1984; Shigeoka et al. 1988; Sangster 1993)

8.63 (Dean 1985)

Molar Volume (cm^3/mol):

145.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

20.93 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$), F: 0.379 (mp at $68^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

9256 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa\cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.37 (Hansch & Leo 1979)

3.05 (HPLC- k' correlation, Hammers et al. 1982)

3.33 (HPLC-RT correlation, Banerjee et al. 1984)

3.47 (shake flask-UV, Beltrame et al. 1984)

3.44, 3.41 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)

3.44 (shake flask, Shigeoka et al. 1988)

3.68 (shake flask/batch equilibration-UV, Beltrame et al. 1988)

3.33 (recommended, Sangster 1993)

3.27; 3.39 (HPLC-RT correlation; electrometric titration, Slater et al. 1994)

3.33 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

1.43, 1.38 (earthworm *E. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)

1.30, 1.61 (earthworm *L. rubellus*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)

1.79, 1.8, 1.94, 2.04 (earthworm system, collated from literature, Connell & Markwell 1990)
 0.8, 1.3, 1.4, 1.80 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

3.09 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 3.03 (2.93–3.13) (soil: organic carbon OC $\geq 0.5\%$ and pH ≤ 6.0 , average, Delle Site 2001)

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

Photolysis:

oxidation:

Hydrolysis:

Biodegradation: biodegradation first-order rate of hydroxylation of 0.008 min^{-1} by *Pseudomonas putida* Fl (Spain et al. 1989; quoted, Neilson et al. 1991).

Biotransformation: degradation rate of $6.84 \times 10^{-19} (\pm 38\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water:

Ground water:

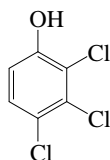
Sediment: mean half-life of dechlorination: $t_{1/2} = 115 \text{ d}$ in July and $t_{1/2} = 86 \text{ d}$ in November with relatively long $t_{1/2} = 66 \text{ d}$ reported from site 1, $t_{1/2} = 64 \text{ d}$ from site 3 and $t_{1/2} = 132 \text{ d}$ from site 5 in January (Hale et al. 1991).

Soil: disappearance $t_{1/2} = 10.1 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 11.2 \text{ d}$ from Holten soil with earthworms *E. fetida andrei* and $t_{1/2} = 24.7 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 49.5 \text{ d}$ from Holten soil with earthworms *L. rebellus* (van Gestel & Ma 1988);

$t_{1/2} = 18.3 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 3.2 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab experiments (Loehr & Matthews 1992).

Biota:

14.1.2.7 2,3,4-Trichlorophenol



Common Name: 2,3,4-Trichlorophenol

Synonym:

Chemical Name: 2,3,4-trichlorophenol

CAS Registry No: 1595-06-0

Molecular Formula: $C_6H_3Cl_3O$, $C_6H_2Cl_3OH$

Molecular Weight: 197.446

Melting Point ($^{\circ}C$):

83.5 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.66 (Doedens 1967)

6.50 (Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984; Shigeoka et al. 1988; Sangster 1993)

6.97 (Ugland et al. 1981; Dean 1985; Renner 1990; Ma et al. 1993)

7.18 (Schellenberg et al. 1984)

Molar Volume (cm^3/mol):

166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\cdot K$, F : 0.267 (mp at $83.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

500 (estimated, Ma et al. 1990)

915 (shake flask-HPLC/UV at pH 5.1, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

1.00 (selected, Ma et al. 1990)

3.48 (selected P_L , Shiu et al. 1994)

Henry's Law Constant ($Pa\cdot m^3/mol$):

0.3959 (calculated- P/C , Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.07 (Hansch & Leo 1979)

3.51 (HPLC-RT correlation, Butte et al. 1981)

3.54 (HPLC- k' correlation, Hammers et al. 1982)

3.80 (shake flask-UV, Beltrame et al. 1984)

3.80 (shake flask, Shigeoka et al. 1988)

3.82 (shake flask/batch equilibration-UV, Beltrame et al. 1988)

3.61 (recommended, Sangster 1993)

3.51, 3.54, 3.80 (lit. values, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants and Half-Lives:

Volatilization:

Photolysis: photochemical-transformation $t_{1/2} = 1.7$ h in Xenotest 1200 (Svenson & Björndal 1988).

Photooxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: 1.7 h for photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988).

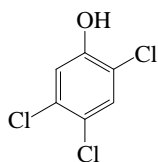
Ground water:

Sediment:

Soil:

Biota:

14.1.2.8 2,4,5-Trichlorophenol



Common Name: 2,4,5-Trichlorophenol

Synonym: 245-TCP

Chemical Name: 2,4,5-trichlorophenol

CAS Registry No: 95-95-4

Molecular Formula: $C_6H_2Cl_3OH$

Molecular Weight: 197.446

Melting Point ($^{\circ}C$):

69 (Lide 2003)

Boiling Point ($^{\circ}C$):

247 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.500 ($75^{\circ}C$, Verschueren 1983)

Acid Dissociation Constant, pK_a :

7.00 (Blackman et al. 1955, Sillén & Martell 1971; Kaiser et al. 1984)

7.07 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

7.43 (Doedens 1967; Jones 1981; Bintein & Devillers 1994)

6.72 (Ugland et al. 1981; Dean 1985; Lagas 1988; Renner 1990; Ma et al. 1993)

6.90 (Hoigné & Bader 1983)

6.94 (Schellenberg et al. 1984; Sangster 1993)

6.83 (Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

166.1 (calculated-Le Bas method at normal boiling point)

165.5 (calculated- χ , Sabljic 1987b)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.59 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.370 (mp at $69^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

948 (shake flask-UV at pH 5.1, Blackman et al. 1955)

990 (IUPAC recommended at pH 5.1, Horvath & Getzen 1985)

700 ($8^{\circ}C$, Leuenberger et al. 1985)

649 (shake flask-HPLC/UV at pH 4.9, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

6.69* (extrapolated-regression of tabulated data, temp range $72-251.8^{\circ}C$, Stull 1947)

6.60 (extrapolated liquid value, Antoine eq, Weast 1972-73)

$\log(P/mmHg) = [-0.2185 \times 13237.0/(T/K)] + 8.401072$; temp range $72-251.8^{\circ}C$ (Antoine eq., Weast 1972-73)

6.12 (supercooled liquid, GC-RT correlation, Hamilton 1980)

2.66 (capillary GC-RT, Bidleman & Renberg 1985)

2.93 (selected, Leuenberger et al. 1985)

7.64 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.38179 - 2812.25/(-2.091 + T/K)$; temp range $345-525 K$ (Antoine eq., Stephenson & Malanowski 1987)

2.93 (calculated, Howard 1991)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.132	(8°C , Leuenberger et al. 1985)
0.590	(calculated, Howard 1991)
0.521	(calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.72	(Leo et al. 1971; Hansch & Leo 1979; 1982)
2.39	(estimated-HPLC-RT correlation, Veith et al. 1979)
3.63	(HPLC- k' correlation, Hammers et al. 1982)
3.80	(shake flask-GC, Saarikoski & Viluksela 1982)
4.19	(shake flask-HPLC/UV, Schellenberg et al. 1984)
4.10, 3.96	(shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
3.73	(HPLC-RT correlation, Miyake et al. 1986)
3.84	(shake flask/batch equilibration-UV, Beltrame et al. 1988)
4.10	(shake flask, Shigeoka et al. 1988)
3.52; 3.55	(shake flask; HPLC-RT correlation, Wang et al. 1989)
3.72	(recommended, Sangster 1993)
4.02	(shake flask-GC, Kishino & Kobayashi 1994)
3.72	(recommended, Hansch et al. 1995)
3.83	(HPLC-RT correlation, Makovskaya et al. 1995b)

Bioconcentration Factor, $\log \text{BCF}$:

3.28	(fathead minnow-28 d exposure, Veith et al. 1979b)
3.28, 2.70	(total ^{14}C in fathead minnows, observed, calculated, mean exposure level $0.0048 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
3.26, 2.82	(total ^{14}C in fathead minnows, observed, calculated, mean exposure level $0.0493 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
3.27	(total ^{14}C in fathead minnows, mean value, Call et al. 1980)
2.40	(calculated- K_{OW} , Mackay 1982)
2.88	(calculated-MCI χ , Sabljic 1987a)
1.79	(fish, van Gestel & Ma 1988)
1.81, 1.53	(earthworms <i>E. fetida andrei</i> : Kooyenburt soil, Holten soil, van Gestel & Ma 1988)
2.04, 2.82	(earthworms <i>L. rubellus</i> : Kooyenburt soil, Holten soil, van Gestel & Ma 1988)
2.04, 2.39, 2.61, 3.36	(earthworm system, collated from literature, Connell & Markwell 1990)
0.40, 1.50, 2.50, 8.40	(earthworm system, derived data, Connell & Markwell 1990)
3.28; 3.61	(fathead minnows; fish, Howard 1991)
2.14	(estimated, NCASI 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

3.49–3.98	(soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
3.38–3.64	(soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
2.56–2.82	(soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
3.38–3.87	(soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
2.55–2.99	(soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
3.36	(sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
2.99	(soil, calculated-MCI χ , Sabljic 1987a,b)
3.25, 3.12, 3.38, 2.56	(quoted:lake sediment, river sediment, aquifer material, soil, Howard 1991)
3.34, 3.30	(soils, Howard 1991)
2.93	(calculated- K_{OW} , Kollig 1993)
3.36	(soil, calculated-MCI χ , Sabljic et al. 1995)
3.11 (2.81–3.41), 3.35 (3.30–3.40)	(soils: organic carbon $\text{OC} \geq 0.1\%$ and $\text{pH} 3.4\text{--}6.0$, $\text{OC} \geq 0.5\%$ and $\text{pH} \leq 4.9$ undissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} \sim 9.0$ d from a model river 1 m deep, flowing 1 m/s with a wind speed of 3 m/s, and $t_{1/2} = 207$ d from a model pond (Howard 1991).

Photolysis:

$k_p = 1.30 \text{ h}^{-1}$ with $t_{1/2} = 0.6$ h in summer at mean temp. 25°C and $k_p = 0.61 \text{ h}^{-1}$ with $t_{1/2} = 1.0$ h in winter at mean temp 18°C in distilled water; $k_p = 1.2 \text{ h}^{-1}$ with $t_{1/2} = 0.6$ d in summer and $k_p = 0.65 \text{ h}^{-1}$ with $t_{1/2} = 1.0$ h in winter in poisoned estuarine water; and $k_p = 1.4 \text{ h}^{-1}$ with $t_{1/2} = 0.5$ h in summer and $k_p = 0.65 \text{ h}^{-1}$ with $t_{1/2} = 1.0$ h in winter for estuarine water under full sunlight and microbes (photo-transformation, Hwang et al. 1986)

$k_p = 1.30 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 0.5$ h in summer, $k_p = 0.61 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 1.0$ h in winter in distilled water and $k_p = 1.20 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 0.6$ h in summer, $k_p = 0.65 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 1.0$ h in winter in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993)

$t_{1/2} = 0.5\text{--}336$ h, based on photolysis rate constants for transformation and mineralization under summer and winter, sunlight conditions (Howard et al. 1991)

photolysis $t_{1/2} = 0.6$ and 1.0 h in natural water (and distilled water) exposed to midday sunlight during summer and winter respectively (Howard 1991)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

aqueous photooxidation $t_{1/2} = 66\text{--}3480$ h in water, based on reported reaction constants for OH and RO_2 radicals with the phenol class (Mill & Mabey 1985; Güesten et al. 1981; selected, Howard et al. 1991)

$k(\text{aq.}) > 10^9 \text{ M}^{-1} \text{ s}^{-1}$ at pH 8, and $k < 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for non-protonated species, $k > 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.2–1.5 and $20\text{--}23^\circ\text{C}$ (Hoigné & Bader 1983b)

$k_{\text{OH}} = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Bunce et al. 1991)

Hydrolysis: $t_{1/2} > 8 \times 10^6$ yr, based on hydrolysis rate constant is zero at pH 7.0 (Kollig et al. 1987; selected, Howard et al. 1991).

Biodegradation: decomposition in suspended soils: > 72 d for complete disappearance (Woodcock 1971; quoted, Verschueren 1983);

840 h for 75% degradation in mineral medium (de Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2} = 552\text{--}16560$ h, based on unacclimated aerobic river die-away test data (Lee & Ryan 1979; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 3028\text{--}43690$ h, based on unacclimated anaerobic grab sample data for soil and ground water (Gibson & Suflita 1986; Baker & Mayfield 1980; selected, Howard et al. 1991);

degradation with microbes in darkness negligible (Hwang et al. 1986);

degradation $k = 0.00010 \text{ d}^{-1}$ with a $t_{1/2} = 16560$ h and $k = 0.030 \text{ d}^{-1}$ with a $t_{1/2} = 552$ h for Skidway River water and water-sediment slurry, respectively (Pritchard 1987);

biodegradation $t_{1/2} = 690$ d in river water (Howard 1991)

70% reduction in concn ($2 \mu\text{M}$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

$t_{1/2}(\text{aerobic}) = 25$ d, $t_{1/2}(\text{anaerobic}) = 130$ d in natural waters (Capel & Larson 1995)

Biotransformation: degradation rate $k = 1.43 \times 10^{-20} (\pm 77\% \text{ SD}) \text{ mol cell}^{-1} \text{ h}^{-1}$ from pure culture studies and $k = 5 \times 10^{-15} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: tropospheric lifetime of 4 d on March 21 at 43°N (Bunce et al. 1991);

$t_{1/2} = 30.1\text{--}301$ h, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

$t_{1/2} \sim 7.5$ d for reactions with OH radical (estimated, Howard 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: 840 h for 75% degradation in mineral medium (de Kreuk & Hanstveit 1981);

Rate constant $k < 3 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with O_3 at pH 1.2–1.5 (Hoigné & Bader 1983);

$t_{1/2} = 0.5$ h (summer), $t_{1/2} = 1.0$ h (winter) in distilled water and $t_{1/2} = 0.5$ h (summer), $t_{1/2} = 1.0$ h (winter) in surface estuarine water based on photo-transformation rate under full sunlight and microbes (Hwang et al. 1986);

- $t_{1/2}$ = 7 d (summer), $t_{1/2}$ = 14 d (winter) in distilled water and $t_{1/2}$ = 3 d (summer), $t_{1/2}$ = 8 d (winter) in estuarine water based on photo-mineralization rate under full sunlight and microbes (Hwang et al. 1986);
- $t_{1/2}$ = 0.6 h (summer), $t_{1/2}$ = 1.0 h (winter) in poisoned estuarine water based on photo-transformation rate and $t_{1/2}$ = 6 d (summer), $t_{1/2}$ = 14 d (winter) in poisoned estuarine water based on photomineralization rate (Hwang et al. 1986);
- $t_{1/2}$ = 16560 h at 21°C in Skidway River water (Pritchard 1987);
- photodegradation $t_{1/2}$ = 0.5 h (summer), $t_{1/2}$ = 1.0 h (winter) in distilled water and $t_{1/2}$ = 0.6 h (summer), $t_{1/2}$ = 1.0 h (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993);
- $t_{1/2}$ = 0.5–336 h, based on aqueous photolysis half-life (Howard et al. 1991); rapidly photolyze with a $t_{1/2}$ = 0.6–1.0 h at water surfaces, $t_{1/2}$ = 690 d in water column (Howard 1991)
- t_2 (aerobic) = 25 d, t_2 (anaerobic) = 130 d in natural waters (Capel & Larson 1995)
- Ground water: $t_{1/2}$ = 1104–43690 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).
- Sediment: $t_{1/2}$ = 23 d from calculated degradation rate constant $k = 0.0030 \text{ d}^{-1}$ for radiolabeled 2,4,5-TCP in Skidway River water-sediment slurry (Lee & Ryan 1979; quoted, Pritchard 1987);
- biodegradation $t_{1/2}$ = 23 d in sediments (Howard 1991).
- Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 + d in Dunkirk silt loam, 47 + d in Mardin silt loam (Alexander & Aleem 1961)
- disappearance $t_{1/2}$ = 3.4 d from Kooyenburg soil and $t_{1/2}$ = 6.6 d from Holten soil with earthworms *E. fetida andrei* and $t_{1/2}$ = 39.6 d from Kooyenburg soil, $t_{1/2}$ = 13.9 d from Holten soil with earthworm *L. rubellus* (van Gestel & Ma 1988);
- $t_{1/2}$ = 33 d in sandy loam (Kjeldsen et al. 1990)
- $t_{1/2}$ = 552–16560 h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991); under aerobic conditions biodegradation $t_{1/2}$ = 15 d in a soil suspension (Howard 1991);
- $t_{1/2}$ = 22.3 d in an acidic clay soil with < 1.0% organic matter and $t_{1/2}$ = 14.6 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).
- Biota: depuration $t_{1/2}$ (obs.) = 12 h, $t_{1/2}$ (calc) = 9.2 h for mean exposure level of $0.0048 \mu\text{g}\cdot\text{mL}^{-1}$ and $t_{1/2}$ (obs) = 12 h, $t_{1/2}$ (calc) = 6.6 h for mean exposure level of $0.0493 \mu\text{g}\cdot\text{mL}^{-1}$ (fathead minnow, Call et al. 1980).

TABLE 14.1.2.8.1**Reported vapor pressures of 2,4,5-trichlorophenol at various temperatures****Stull 1947****summary of literature data**

t/°C	P/Pa
72.0	133.3
102.1	666.6
117.3	1333
134.0	2666
151.5	5333
162.5	7999
178.0	13332
201.5	26664
226.5	53329
251.8	101325
mp/°C	62

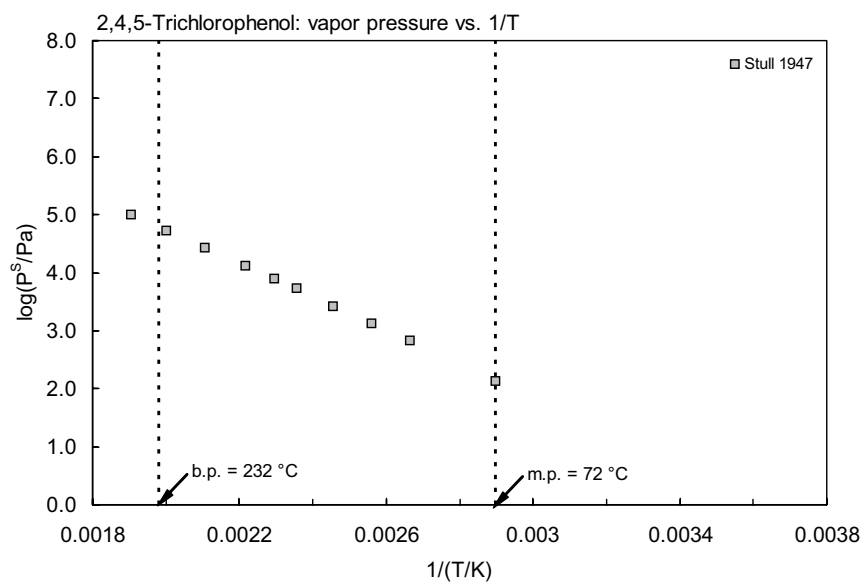
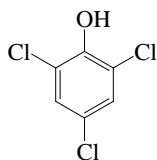


FIGURE 14.1.2.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2,4,5-trichlorophenol.

14.1.2.9 2,4,6-Trichlorophenol



Common Name: 2,4,6-Trichlorophenol

Synonym: 2,4,6 TCP

Chemical Name: 2,4,6-trichlorophenol

CAS Registry No: 88-06-2

Molecular Formula: $C_6H_2Cl_3OH$

Molecular Weight: 197.446

Melting Point ($^{\circ}C$):

69 (Lide 2003)

Boiling Point ($^{\circ}C$):

246.0 (Stull 1947; Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.675 (Schmidt-Bleek et al. 1982)

1.491 ($75^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

6.10 (Blackman et al 1955)

6.22 (Farquharson et al. 1958; Saarikoski & Viluksela 1982)

5.99 (Dean 1985)

6.23 (Serjeant & Dempsey 1979; Tratnyek & Hoigné 1991)

6.00 (Xie 1983, Yoshida et al. 1987)

6.15 (Schellenberg et al. 1984; Leuenberger et al. 1985)

6.18 (Sangster 1993)

Molar Volume (cm^3/mol):

166.1 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.370 (mp at $69^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

858 (gravimetric method, Dacomo 1885)

434 (shake flask-UV at pH 5.1, Blackman et al. 1955)

900 (shake flask-spectrophotometry, Roberts et al. 1977)

430 (IUPAC recommended at pH 5.1, Horvath & Getzen 1985)

312 ($20^{\circ}C$, phenol form, shake flask-HPLC/UV, Yoshida et al. 1987)

$312 \times (1 + 10^{pH-6.06})$ ($20^{\circ}C$, measured at pH 4, 5, 6 and 7, shake flask-HPLC/UV, Yoshida et al. 1987)

300, 580, 270000 (river, oligotrophic lake, eutrophic lake, Yoshida et al. 1987)

708 (shake flask-HPLC/UV at pH 4.7, Ma et al. 1993)

800 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

692* ($24.9^{\circ}C$, shake flask-conductimetry, measured range 19.5 – $30.0^{\circ}C$, Achard et al. 1996)

1144* ($41.05^{\circ}C$, shake flask-optical method, measured range 314.2 – $420.6 K$, Jaoui et al. 1999)

503 (shake flask-HPLC/UV, pH 5.03, Huang et al. 2000)

439.6* ($21.75^{\circ}C$, shake flask-optical method, measured range 294.9 – $317.2 K$, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 23.367 - 7096.7/(T/K)$; temp range 292 – $303 K$ (eq. derived using reported exptl. data, Jaoui et al. 2002)

$\ln [S/(mol kg^{-1})] = 6.6069 - 2029.9/(T/K)$; temp range 303 – $334 K$ (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 4.17* (extrapolated-regression of tabulated data, temp range 76.5–246°C, Stull 1947)
- 4.00 (20–25°C, extrapolated, Jordan 1954)
- 4.12 (extrapolated liquid, Antoine eq., Weast 1972–73)
- $\log(P/\text{mmHg}) = [-0.2185 \times 14092.8/(T/K)] + 8.82338$; temp range 76.5–246°C (Antoine eq., Weast 1972–73)
- 3.83 (supercooled liquid, GC-RT correlation, Hamilton 1980)
- 1.12 (gas saturation, Politzki et al. 1982)
- 1.30 (20°C, Schmidt-Bleek et al. 1982)
- 1.60 (extrapolated, Mabey et al. 1982)
- 2.67 (Leuenberger et al. 1985)
- 3.26 (capillary GC-RT correlation, supercooled liquid P_L , Bidleman & Renberg 1985)
- 4.28 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 7.67323 - 2876.7/(-11.682 + T/K)$, temp range 349–519 K (Antoine eq., Stephenson & Malanowski 1987)
- 0.827 (GC-RT correlation, solid phase, Yoshida et al. 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C or as indicated):

- 0.405 (calculated-P/C, Mabey et al. 1982)
- 0.132 (8°C, calculated-P/C, Leuenberger et al. 1985)
- $0.523/(1 + 10^{\text{pH} + 6.06})$ (20°C, calculated-P/C, Yoshida et al. 1987)
- 0.5687 (calculated-P/C, Shiu et al. 1994)
- 0.428 (20°C, single equilibrium static technique SEST, Sheikheldin et al. 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.06 (Leo et al. 1971)
- 3.69 (Leo et al. 1971)
- 3.69, 3.62, 4.02 (Hansch & Leo 1979)
- 3.76 (HPLC-RT correlation, Butte et al. 1981)
- 3.48 (RP-HPLC- k' correlation, Miyake & Terada 1982)
- 4.03 (shake flask-GC, Saarikoski & Viluksela 1982)
- 3.72 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 2.97, 2.80 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
- 3.75, 3.69 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
- 3.72 (OECD 1981 guidelines, Leuenberger et al. 1985)
- 3.29 (RP-HPLC-RT correlation, Chin et al. 1986)
- 3.97 (CPC-RV, Terada et al. 1987)
- 3.75 (HPLC-RT correlation, Shigeoka et al. 1988)
- 3.68 (batch equilibration-UV, Beltrame et al. 1988)
- 3.96; 3.60 (shake flask; HPLC-RT correlation, Wang et al. 1989)
- 3.69 (recommended, Sangster 1993)
- 2.67 (shake flask-GC, Kishino & Kobayashi 1994)
- 3.69 (recommended, Hansch et al. 1995)
- 3.84, 3.76, 3.65, 3.54 (pH 3.0, 6.1, 7.0, 8.0, shake flask-GC (octanol phase)/HPLC (aqueous phase) measured range pH 2.1 to 13.3, Nowosielski & Fein 1998)

Bioconcentration Factor, $\log BCF$:

- 2.00–2.32 (Landner et al. 1977; Laake 1982)
- 2.40 (fish, Körte et al. 1978)
- 1.60, 1.71, 2.49 (activated sludge, algae, golden orfe, Freitag et al. 1982)
- 1.71; 1.81 (algae: exptl; calculated, Geyer et al. 1981)
- 1.54–1.78, 1.60 (mussel *mytilus edulis*, Geyer et al. 1982)
- 2.92 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 3.24, 3.48, 3.1–4.09 (algae, snail, guppy, Virtanen & Hattula 1982)
- 1.71, 2.49, 1.60 (algae, fish, activated sludge, Klein et al. 1984)

- 1.71, 2.13 (algae: exptl., calculated- K_{OW} , Geyer et al. 1984)
 1.78, 1.70, 2.49 (activated sludge, algae, golden ide, Freitag et al. 1985)
 1.48–2.08 (rainbow trout, Oikari et al. 1985)
 2.75; 2.84 (Atlantic salmon fry: humic water; lake water, Carlberg et al. 1986)
 1.30 (Isnard & Lambert 1988)
 1.94; 2.83 (flagfish: whole fish; fish lipid, Smith et al. 1990)
 1.87–2.16 (estimated, NCASI 1992)
 1.48–2.08, 3.01–4.09, 2.49, 3.48, 1.60, 1.70–3.24 (trout, guppy, fish, snail, mussel, algae, quoted from literature, NCASI 1992)
 3.6, 5.4, 5.0 (perch bile to water, Söderström et al. 1994)
 2.84 (*Salmo salar*, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

- 2.34 (sediment, Virtanen & Hattula 1982)
 3.30 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 2.52 (soil, Seip et al. 1986)
 3.41–3.84 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 3.33–3.57 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 2.52–2.75 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 3.30–3.73 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 2.48–2.87 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 3.02 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
 3.03 (sediment, Leuenberger et al. 1985)
 2.99 (soil, calculated, Sabljic 1987a,b)
 3.34, 2.79, 2.23 (average values, soil at pH 6, 7, and 7.7, Yoshida et al. 1987)
 2.79, 3.34, 2.04 (river, oligotrophic lake, eutrophic lake, Yoshida et al. 1987)
 2.50 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
 2.92–3.12; 3.03 (lit. range, mean value, Robinson & Novak 1994)
 2.82–3.02 (log K_{OM} , organic matter, Robinson & Novak 1994)
 2.81, 3.03 (log K_{HA} , humic acid, Robinson & Novak 1994)
 2.25 (calculated- K_{OW} , Kollig 1993)
 3.02 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.59; 3.08 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 2.52 (1.97–3.01), 2.88 (2.33–3.39) (soils: organic carbon OC \geq 0.1% and pH $>$ 4.2, OC \geq 0.1% and pH \leq 4.2 undissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: volatilization and sorption $t_{1/2} \sim 192$ h from natural pond (Schauerte et al. 1982);
 volatilization rate constant from water $k = 3.90 \times 10^{-3} / (1 + 10^{pH-6.06}) / L_w$ h $^{-1}$, L_w , depth of water phase (Yoshida et al. 1987).
 Photolysis: aqueous photolysis $t_{1/2} = 2$ –96 h, based on laboratory photolysis rate constants for an environmental pond at noon under fall sunlight conditions at 40°N latitude (Sugiura et al. 1984; quoted, Howard et al. 1991);
 photo-degradation rate constants $k_p = (0.156 + 9.16 \times 10^{pH-5.86}) / (1 + 10^{pH-5.86})^{-1}$ in water, for summer, fine day, and $k_p = (0.042 + 1.40 \times 10^{pH-6.09}) / ((1 + 10^{pH-6.09})^{-1})$ h $^{-1}$ in water, for winter, fine day; $k = 0.72$ d $^{-1}$ for river, $k = 2.2$ d $^{-1}$ for oligotrophic lake and $k = 0.776$ d $^{-1}$ for eutrophic lake (Yoshida et al. 1987);
 photochemical-transformation $t_{1/2} = 1.2$ h in Xenotest 1200 (Svenson & Björndal 1988);
 photolysis $t_{1/2} = 24$ h (Paasivirta 1992);
 photo-degradation rate constant $k = 26 \times 10^3$ min $^{-1}$ with $t_{1/2} = 25.2$ min for direct UV radiation aqueous solutions (Benitez et al. 2000).
 Oxidation: aqueous oxidation rate constant $k < 7 \times 10^4$ M $^{-1}$ h $^{-1}$ for singlet oxygen and $k = 1 \times 10^6$ M $^{-1}$ h $^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);
 apparent reaction rate constant $k > 10^8$ M $^{-1}$ s $^{-1}$ at pH 8, and rate constants $k < 10^4$ M $^{-1}$ s $^{-1}$ for non-protonated species, $k > 10^8$ M $^{-1}$ s $^{-1}$ for phenolate ions for the reaction with ozone in water using 3 mM *t*-BuOH as scavenger at pH 1.3–1.5 and 20–23°C (Hoigné & Bader 1983b);

photooxidation $t_{1/2} = 123.4\text{--}1234$ h, based on an estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; quoted, Howard et al. 1991);

photooxidation $t_{1/2} = 20.3\text{--}2027$ h, based on measured rate data for reaction with singlet oxygen in aqueous solution (Scully & Hoigne 1987; quoted, Howard et al. 1991);

rate constants: $k = 2 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.2, $k = 6 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 4.8, $k = 1.5 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.2, $k = 2.6 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 5.5, $k = 5.5 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 6.0, $k = 9.50 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7 and $k = 1.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$ at pH 9 for the reaction with singlet oxygen in aqueous solution at $(19 \pm 2)^\circ\text{C}$ (Scully & Hoigné 1987);

rate constant $k = (1.7 \pm 0.7) \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991);

photo-oxidation rate constant $k = 98 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 5.1$ min for reaction with Fenton's reagent; and $k = 44 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 20.6$ min at pH 2 and $k = 314 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 3.1$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Hydrolysis: $t_{1/2} > 8 \times 10^6$ yr, based on hydrolysis rate constant of zero at pH 7 (Kollig et al. 1987; quoted, Howard et al. 1991).

Biodegradation: $t_{1/2} = 7\text{--}10$ d for bacteria to utilize 95% of 300 ppm in parent substrate (Tabak et al. 1964); decompositions in soil suspensions: 5 d for complete disappearance (Woodcock 1971; quoted, Verschueren 1983); $t_{1/2} = 216\text{--}432$ h and $624\text{--}1560$ h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981);

aqueous aerobic $t_{1/2} = 168\text{--}1680$ h, based on unacclimated aerobic river die-away test and soil grab sample data (Blades-Fillmore et al. 1982; Haider et al. 1974; quoted, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 4050\text{--}43690$ h, based on unacclimated anaerobic grab sample data for soil (Baker & Mayfield 1980; quoted, Howard et al. 1991);

92% aerobic biodegraded after 28 d by both Sturm of OECD and sealed vessel tests (Birch & Fletcher 1991);

biodegradation rate constant $k = 3.5 \times 10^{-11} \text{ L cell}^{-1} \text{ h}^{-1}$ at 20°C and pH 7;

biodegradation rate constants $k = 8.4 \times 10^{-5} \text{ d}^{-1}$ in river, $k = 8.2 \times 10^{-6} \text{ d}^{-1}$ in oligotrophic lake and $k = 8.4 \times 10^{-4} \text{ d}^{-1}$ in eutrophic lake in water compartment, $k = 8.4 \times 10^{-4} \text{ d}^{-1}$ in river, $k = 8.2 \times 10^{-5} \text{ d}^{-1}$ in oligotrophic lake and $k = 8.4 \times 10^{-3} \text{ d}^{-1}$ in eutrophic lake in soil compartment (Yoshida et al. 1987);

94% reduction in concn (2 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

up to 60% can be mineralized by acclimated bacteria *pseudomonas aeruginosa* in 48 h but decreased with increasing humic acid concentration (Robinson & Novak 1994)

Degradation constant $k = 3.2\text{-M/h}$ for anaerobic batch experiment in serum bottles; $k = 2.4 \text{-M/h}$ for dechlorination in anaerobic batch or continuous bioreactor; $k = 2.4 \text{-M/h}$ in the sequential anaerobic-aerobic continuous reactor system (Armenante et al. 1999)

Biotransformation: rate constant for bacterial transformation $k = 3 \times 10^9 \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 421 \text{ d}^{-1}$, 3573 d^{-1} (flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 4.78 \text{ d}^{-1}$, 5.26 d^{-1} (flagfish: whole fish, fish lipid, Smith et al. 1990)

$k_2 = 4.78 \text{ d}^{-1}$, 2.54 d^{-1} (fish: bioconcentration based; toxicity based, Smith et al. 1990)

Half-Lives in the Environment:

Air: $t_{1/2} = 123.4\text{--}1234$ h, based on an estimated rate constant for the vapor phase reaction with OH radical (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $> 5\text{d}$ (Kelly et al. 1994).

Surface water: $t_{1/2} = 216\text{--}432$ h and $624\text{--}1560$ h for 75% degradation in mineral medium and seawater batch experiment, respectively (de Kreuk & Hanstveit 1981);

$t_{1/2} = 1.2$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2} = 2\text{--}96$ h, based on aqueous photolysis half-life (Sugiura et al. 1984; quoted, Howard et al. 1991);

$t_{1/2} = 62$ h for the reaction with singlet oxygen at pH 8 and $(19 \pm 2)^\circ\text{C}$ in water (Scully & Hoigné 1987)

photolysis $t_{1/2} = 24$ h (Paasivirta 1992);

photo-oxidation $t_{1/2} = 5.1$ min for reaction with Fenton's reagent; $t_{1/2} = 20.6$ min at pH 2 and $t_{1/2} = 3.1$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{1/2}$ = 336–43690 h, based on estimated unacclimated aqueous aerobic biodegradation half-life and aqueous anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 5 d in Dunkirk silt loam, 13 d in Mardin silt loam (Alexander & Aleem 1961)

$t_{1/2}$ = 168–1680 h, based on estimated unacclimated aqueous aerobic biodegradation half-life including soil grab sample data (Haider et al. 1974; quoted, Howard et al. 1991);

$t_{1/2}$ = 6.3 d in an acidic clay soil with < 1.0% organic matter and $t_{1/2}$ = 5.3 d in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch laboratory microcosm experiments (Loehr & Matthews 1992);

$t_{1/2}$ = 6720 h (Paasivirta 1992).

Biota: $t_{1/2}$ = 0.15 d of clearance from whole flagfish; $t_{1/2}$ = 0.13 d of clearance from flagfish lipid (Smith et al. 1990).

TABLE 14.1.2.9.1

Reported aqueous solubilities and vapor pressures of 2,4,6-trichlorophenol at various temperatures

Aqueous solubility						Vapor pressure	
Achard et al. 1996		Jaoui et al. 1999		Jaoui et al. 2002		Stull 1947	
shake flask-conductivity		shake flask-optical method		shake flask-optical method*		summary of literature data	
t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³	T/K	S/g·m ⁻³	t/°C	P/Pa
19.5	410	314.2	1144	294.9	493.6	76.5	133.3
20.1	427	334.3	1376	304.6	947.8	105.9	666.6
24.9	692	335.3	1377	308.6	933.1	120.2	1333
30.0	928	337.6	1733	314.6	1362	135.8	2666
		342.3	2116	320.9	1323	152.2	5333
		345.3	2377	294.9	493.6	163.5	7999
		352.2	2832	297.7	631.8	177.8	13332
		369.9	3391	302.4	908.3	199.0	26664
		383.8	5419	307.5	1007	222.5	53329
		408.1	7086	313.7	1145	246.0	101325
		420.6	7777	292.8	414.6		
				302.2	888.5	mp/°C	68.5
				308.0	1007		
				317.2	1224		
some data from Achard et al. 1996, Jaoui et al. 1999							

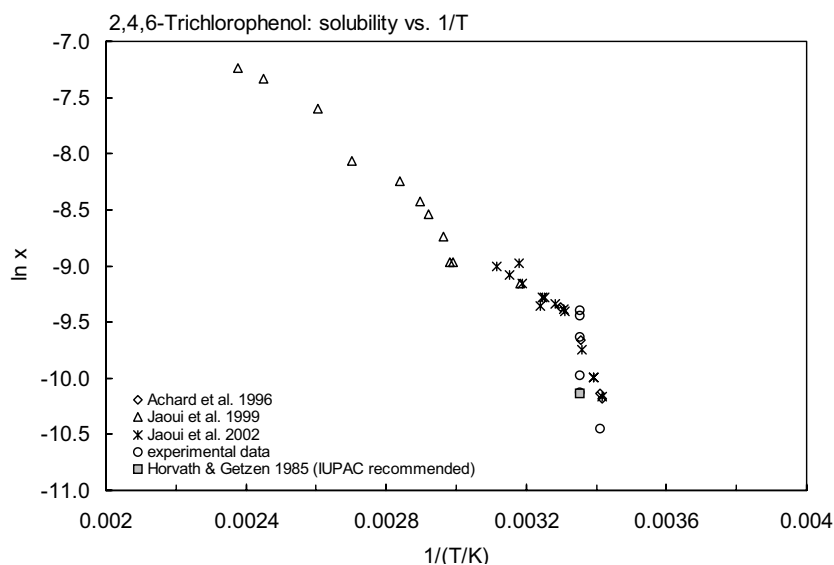


FIGURE 14.1.2.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,4,6-trichlorophenol.

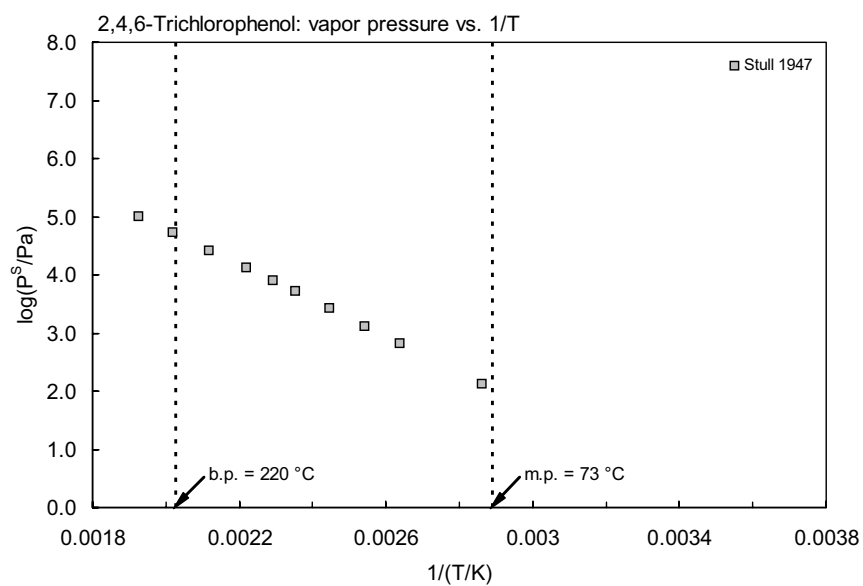
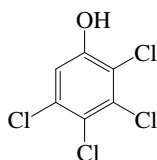


FIGURE 14.1.2.9.2 Logarithm of vapor pressure versus reciprocal temperature for 2,4,6-trichlorophenol.

14.1.2.10 2,3,4,5-Tetrachlorophenol



Common Name: 2,3,4,5-Tetrachlorophenol

Synonym:

Chemical Name: 2,3,4,5-tetrachlorophenol

CAS Registry No: 4901-51-3

Molecular Formula: C_6HCl_4OH

Molecular Weight: 231.891

Melting Point ($^{\circ}C$):

116.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.96 (Doedens 1967)

5.30 (Sillén & Martell 1971; Kaiser et al. 1984)

5.64 (Könemann 1981; Könemann & Musch 1981; Ugland et al. 1981; Dean 1985; Renner 1990)

6.35 (Schellenberg et al. 1984)

6.61 (Xie & Dyrssen 1984)

6.12 (Nendza & Seydel 1988)

6.48 (Sangster 1993)

Molar Volume (cm^3/mol):

187.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.127 (mp at $116.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

166 (shake flask-HPLC/UV at pH 4.9, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol):

0.140 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.95 (Hansch & Leo 1979)

5.03 (HPLC-RT correlation, Banerjee et al. 1984)

4.21 (shake flask-UV, Beltrame et al. 1984)

4.87 ($20^{\circ}C$, shake flask-HPLC, Schellenberg et al. 1984)

4.82, 4.68 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)

4.71 (shake flask-GC, Xie & Dyrssen 1984)

4.54 (batch equilibration-UV, Beltrame et al. 1988)

4.21 (recommended, Sangster 1993)

4.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

- 1.61, 1.60 (earthworm *E. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
 2.55, 2.33 (earthworm *L. rubellus*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
 2.61, 2.73, 3.49, 3.53 (earthworm system, collated from literature, Connell & Markwell 1990)
 0.40, 0.50, 2.30, 4.10 (earthworm system, derived data, Connell & Markwell 1990)

Sorption Partition Coefficient, log K_{OC} :

- 4.21–4.66 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 3.77–4.01 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 2.94–3.17 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 4.11–4.55 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 3.20–3.60 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 4.12 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
 3.32 (soil, calculated-MCI χ , Sabljic 1987a,b)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: photochemical transformation $t_{1/2} = 0.88$ h in Xenotest 1200 (Svenson & Björndal 1988).

Oxidation:

Hydrolysis:

Biodegradation: 100% reduction in concn (2 μ M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation: degradation rate constant $k = 7.14 \times 10^{-22}$ ($\pm 41\%$ SD) $\text{mol}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ from pure culture studies and $k = 5 \times 10^{-16}$ $\text{mol}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: $t_{1/2} = 0.88$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988).

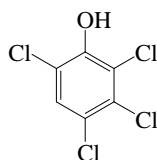
Ground water:

Sediment:

Soil: disappearance $t_{1/2} = 43.4$ d from Kooyenburg soil, $t_{1/2} = 29.1$ d from Holten soil with earthworm *E. fetida andrei* and $t_{1/2} = 26.8$ d from Kooyenburg soil, $t_{1/2} = 42.5$ d from Holten soil with earthworm *L. rebellus* (van Gestel & Ma 1988).

Biota:

14.1.2.11 2,3,4,6-Tetrachlorophenol



Common Name: 2,3,4,6-Tetrachlorophenol

Synonym:

Chemical Name: 2,3,4,6-tetrachlorophenol

CAS Registry No: 58-90-3

Molecular Formula: C_6HCl_4OH

Molecular Weight: 231.891

Melting Point ($^{\circ}C$):

70.0 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

150 (at 15 mm Hg, Weast 1982–83)

Density (g/cm^3):

1.60 (at $60^{\circ}C$, Verschueren 1983)

Acid Dissociation Constant, pK_a :

5.40 (Blackman et al. 1955; Xie 1983; Schellenberg et al. 1984; Sangster 1993)

5.46 (Farquharson et al. 1958; Saarikoski & Viluksela 1982; Renner 1990)

5.30 (Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)

5.22 (Ugland et al. 1981; Dean 1985; Lagas 1988; Renner 1990; Ma et al. 1993)

5.62 (Xie & Dyrssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)

Molar Volume (cm^3/mol):

187.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} , (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.362 (mp at $70^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

183 (shake flask-UV at pH 5.1, Blackman et al. 1955)

180 (recommended at pH 5.1, IUPAC Solubility Data Series, Horvath & Getzen 1985)

166 (shake flask-HPLC/UV, pH 4.62, Huang et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.763 (extrapolated-regression of tabulated data, temp range 100 – $275^{\circ}C$, Stull 1947)

0.750 (extrapolated liquid, Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 15362.7/(T/K)] + 9.016052$; temp range 100 – $275^{\circ}C$ (Antoine eq., Weast 1972–73)

0.692 (supercooled liq. value, GC-RT correlation, Hamilton 1980)

0.564 (capillary GC-RT correlation, Bidleman & Renberg 1985)

0.810 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.96172 - 3227.92/(-6.121 + T/K)$; temp range 373 – $548 K$ (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa m^3/mol$):

0.3548 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.10 (Hansch & Leo 1979)

4.27 (RP-HPLC- k' correlation, Miyake & Terada 1982)

4.45 (shake flask-GC, Saarikoski & Viluksela 1982)

- 4.12 (shake flask-UV, Beltrame et al. 1984)
- 4.42 (shake flask-HPLC/UV, Schellenberg et al. 1984)
- 4.42, 4.34 (shake flask-GC, HPLC- k' correlation, Xie et al. 1984)
- 4.31 (shake flask-GC, Xie & Dyrssen 1984)
- 4.42 (OECD 1981 guidelines, Leuenberger et al. 1985)
- 4.25 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
- 4.42 (shake flask, Shigeoka et al. 1988)
- 4.37 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
- 4.45 (recommended, Sangster 1993)
- 4.24 (shake flask-GC, Kishino & Kobayashi 1994)
- 4.45 (recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

- 2.65 (trout, Hattula et al. 1981)
- 2.55–2.69 (estimated, NCASI 1992)
- 3.3, 3.8, 4.4, 4.5 (perch bile to water, Söderström et al. 1994)

Sorption Partition Coefficient, log K_{OC} :

- 4.21 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
- 3.77 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
- 2.94 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
- 4.11 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
- 3.20 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
- 3.82 (sediment, Schellenberg et al. 1984; quoted, Sabljic 1987a,b)
- 3.35 (soil, Seip et al. 1986; quoted, Sabljic 1987a,b)
- 3.32 (soil, calculated-MCI χ , Sabljic 1987a,b)
- 3.90 (calculated, Lagas 1988)
- 2.45, 2.70 (totally dissociated as phenolate-calculated, Lagas 1988)
- 3.35 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
- 3.02 (2.35–3.69), 3.06 (2.31–3.81), 3.75(3.69–3.81), 2.28(2.16–2.40) (soils: organic carbon $OC \geq 0.1\%$ and pH 3.4–7.5, $OC \geq 0.5\%$, $OC \geq 0.5\%$ pH ≤ 3.4 undissociated, $OC \geq 0.5\%$ pH ≥ 7.4 dissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: aqueous photolysis $t_{1/2} \sim 1$ –336 h, based on aqueous data for 2,4,5- 2,4,6-trichlorophenols and pentachlorophenol (Howard et al. 1991);
photo-degradation rate constant $k = 21 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 30.6 \text{ min}$ for direct UV radiation aqueous solutions (Benitez et al. 2000).

Photooxidation: atmospheric $t_{1/2} = 364.4$ –3644 h, based on estimated rate constant for reaction with OH radical and aqueous $t_{1/2} = 66.0$ –3480 h, based on reaction rate constants with OH and $RO_2\cdot$ radicals with phenol class (Howard et al. 1991);

photo-oxidation rate constant $k = 9 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 49.5 \text{ min}$ for reaction with Fenton's reagent; and $k = 94 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 10.6 \text{ min}$ at pH 2 and $k = 415 \times 10^3 \text{ min}^{-1}$ with $t_{1/2} = 1.9 \text{ min}$ at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Hydrolysis: no hydrolyzable groups (Howard et al. 1991).

Biodegradation: decomposition in soil suspensions: $t_{1/2} > 72 \text{ d}$ for complete disappearance (Woodcock 1971; quoted, Verschuere 1983);

aqueous aerobic $t_{1/2} = 672$ –4032 h, based on acclimated aerobic screening test data and aqueous anaerobic $t_{1/2} = 2688$ –16128 h, based on unacclimated aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 364.4\text{--}3644$ h, based on estimated photooxidation half-life in air (Howard et al. 1991).

Surface water: $t_{1/2} = 0.88$ h, based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);

$t_{1/2} = 1\text{--}336$ h, based on estimated aqueous photolysis data for trichlorophenols and PCP (Howard et al. 1991);

photo-oxidation $t_{1/2} = 49.5$ min for reaction with Fenton's reagent; $t_{1/2} = 10.6$ min at pH 2, and $t_{1/2} = 1.9$ min at pH 9 for reactions with ozone in aqueous solutions (Benitez et al. 2000).

Ground water: $t_{1/2} = 1344\text{--}8640$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

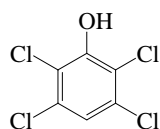
Sediment:

Soil: Days for complete disappearance by microbial decomposition in soil suspension: 72 ± 2 d in Dunkirk silt loam (Alexander & Aleem 1961)

$t_{1/2} = 672\text{--}4320$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

14.1.2.12 2,3,5,6-Tetrachlorophenol



Common Name: 2,3,5,6-Tetrachlorophenol

Synonym:

Chemical Name: 2,3,5,6-tetrachlorophenol

CAS Registry No: 935-95-5

Molecular Formula: $C_6H_2Cl_4O$, C_6HCl_4OH

Molecular Weight: 231.891

Melting Point ($^{\circ}C$):

115 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

5.30 (Sillen & Martell 1971)

5.03 (Konemann 1981; Ugland et al. 1981)

5.40 (Sangster 1993)

Molar Volume (cm^3/mol):

187.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.131 (mp at $115^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

100 (shake flask-HPLC/UV, pH 5.0, Ma et al. 1993)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.90 (Hansch & Leo 1979)

4.42 (calculated-fragment constant, Konemann 1981)

4.88 (HPLC-RT correlation, Butte et al. 1981)

3.88 (shake flask-UV, Beltrame et al. 1984)

4.47 (HPLC-RT correlation, Xie et al. 1984)

3.88 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$, or Lifetimes, τ :

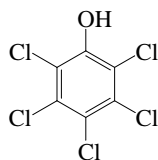
Biodegradation: 100% reduction in concn ($2 \mu M$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

Half-Lives in the Environment:

14.1.2.13 Pentachlorophenol



Common Name: Pentachlorophenol

Synonym: chlorophen, PCP, penchlorol

Chemical Name: pentachlorophenol

CAS Registry No: 87-86-5

Molecular Formula: C_6Cl_5OH

Molecular Weight: 266.336

Melting Point ($^{\circ}C$):

191.0 (Firestone 1977; Weast 198–83)

174 (Lide 2003)

Boiling Point ($^{\circ}C$):

309–310 (dec., Weast 1982–83)

310 (dec., Lide 2003)

Density (g/cm^3):

1.987 (Firestone 1977)

1.978 (22 $^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

4.80 (Blackman et al. 1955; Sillén & Martell 1971; McLeese et al. 1979; Kaiser et al. 1984)

5.00 (Farquharson et al. 1958; Renner 1990)

4.74 (Drahonovsky & Vacek 1971)

4.71 (spectrophotometric, Cessna & Grover 1978)

5.20 (Renberg 1981; Renner 1990; Larsson et al. 1993)

5.25 (Schellenberg et al. 1984)

4.90 (Xie & Dyrssen 1984; Xie et al. 1986; Shigeoka et al. 1988; Söderström et al. 1994)

4.60 (Nendza & Seydel 1988)

Molar Volume (cm^3/mol):

207.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.5 (exptl., Chickos et al. 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, F: 0.0350 (mp at 174 $^{\circ}C$))

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

15.4* (gravimetric method, measured range 0–70 $^{\circ}C$, Carswell & Nason 1938)

18.0 (27 $^{\circ}C$, gravimetric method, Carswell & Nason 1938)

9.59 (shake flask-UV, at pH 5.1, Blackman et al. 1955)

14.0 (20 $^{\circ}C$, shake flask-UV, at pH 3.0, Bevenue & Beckman 1967)

10.0 (shake flask-gravimetric, at pH 5.0, Toyota & Kuwahara 1967)

14.0 (gravimetric at pH 5.0, Toyota & Kuwahara 1967)

5–10 (at pH 5–6 in contaminated water, Goerlitz et al. 1985)

14.0 (IUPAC recommended at pH 4.5–5.5, Horvath & Getzen 1985)

8.0 \pm 2 (shake flask-UV at pH 2.5, Valsaraj et al. 1991)

32 \pm 3 (shake flask-UV at pH 5.0, Valsaraj et al. 1991)

18.4 (shake flask-HPLC/UV, at pH 4.8, Ma et al. 1993)

5.0 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

21.4* (25.1 $^{\circ}C$, shake flask-conductimetry, measured range 25.1–46.8 $^{\circ}C$, Achard et al. 1996)

- 13.0 (shake flask-HPLC/UV, pH 4.55, Huang et al. 2000)
 102* (60.05°C, shake flask-optical method, measured range 333.2–422.3 K, Jaoui et al. 1999)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.0227* (20°C, extrapolated-static method, measured range 100–220°C, Carswell & Nason 1938)
 2666* (192.2°C, summary of literature data, temp range 192.2–309.3°C, Stull 1947)
 0.108* (46.0°C, ebulliometry, measured range 46.0–233.87°C, McDonald et al. 1959)
 0.0147–0.0227 (20°C, Goll 1954; Bevenue & Beckman 1967; Neumüller 1974)
 0.0147 (20°C, Bevenue & Beckman 1967)
 0.100 (extrapolated-Antoine eq., Weast 1972–73)
 $\log(P/\text{mmHg}) = [-0.2185 \times 16742.6/(T/K)] + 9.150200$; temp range 192.2–309.3°C (Antoine eq., Weast 1972–73)
 0.231 (supercooled liq. extrapolated-Antoine eq., Weast 1976–77; quoted, Bidleman & Renberg 1985)
 0.0213 (Firestone 1977)
 0.0956 (supercooled liquid, GC-RT correlation, Hamilton 1980)
 0.00415 (23°C, OECD, Klöpffer et al. 1982)
 0.1153 (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 7.22246 - 2846.009/(230.158 + t/^\circ\text{C})$, temp range 200–253°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 0.115 (capillary GC-RT, supercooled liquid P_L , Bidleman & Renberg 1985)
 0.127 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.198 - 3606/(T/K)$, temp range 463–507 K (Antoine eq., Stephenson & Malanowski 1987)
 0.0070* (gas saturation-GC, measured range 25–125°C, Rordorf 1989)
 0.0147 (Howard 1991)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 0.284 (calculated-P/C, Mabey et al. 1982)
 0.0025 (calculated-P/C, Hellmann 1987)
 0.0127 (estimated-bond contribution, Hellmann 1987)
 0.277 (calculated-P/C, Howard 1991)
 0.079 (calculated-P/C, Shiu et al. 1994)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 5.01 (Leo et al. 1971)
 3.81 (Lu & Metcalf 1975)
 5.01, 5.12, 5.86, 3.81 (lit. values, Hansch & Leo 1979)
 5.01 (HPLC-RT correlation, Veith et al. 1979b)
 5.10 (HPLC- k' correlation, Butte et al. 1981)
 4.00 (at pH 4, Renberg 1981)
 5.08 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 5.15 (shake flask-GC, Saarikoski & Viluksela 1982; Saarikoski et al. 1986)
 4.84 (shake flask-GC, apparent value at pH 1.2, Kaiser & Valdmanis 1982)
 1.30 (shake flask-GC, apparent value at pH 10.5, Kaiser & Valdmanis 1982)
 3.69 (Geyer et al. 1982, Schmidt-Bleek et al. 1982)
 3.29 (shake flask average, OECD/EEC Lab. comparison tests, Harnish et al. 1983)
 5.11 ± 0.07 (HPLC-retention volume correlation-ALPM, Garst & Wilson 1984)
 3.69, 3.81 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
 5.24 (shake flask-HPLC/UV, Schellenberg et al. 1984)
 5.04, 5.08 shake flask-GC, HPLC- k' , Xie et al. 1984)
 5.12 (Hansch & Leo 1985)
 5.24 (OECD 1981 guidelines, Leuenberger et al. 1985)
 4.71 (RP-HPLC-RT correlation, Chin et al. 1986)
 2.50 (at pH 4.7, Geyer et al. 1987)
 4.47 (centrifugal partition chromatography CPC-RV, Terada et al. 1987)
 5.04 (HPLC-RT correlation, Shigeoka et al. 1988)

- 5.00 (shake flask/batch equilibration-UV, Beltrame et al. 1988)
- 5.18 (recommended, LOGKOW databank, Sangster 1993)
- 5.06, 5.12 (COMPUTOX databank, Kaiser 1993)
- 5.02 (shake flask-GC/ECD, Kishino & Kobayashi 1994)
- 5.12 (recommended, pH 1.4, Hansch et al. 1995)
- 4.74, 4.60, 4.27, 3.69, 3.59 (pH 2.1–3.1, 5.0, 6.1, 7.2, 8.0, shake flask-GC (octanol phase)/HPLC (aqueous phase), measured range pH 2.1–13.3, Nowosielski & Fein 1998)

Bioconcentration Factor, log BCF:

- 3.75 (fish, Statham et al. 1976)
- 3.04 (fish, Körte et al. 1978)
- 2.89 (fathead minnow, Veith et al. 1979)
- 2.89 (fathead minnow, calculated value, Veith et al. 1979b)
- 3.09, 2.64 (algae: exptl., calculated, Geyer et al. 1981)
- 2.00 (trout, Hattula et al. 1981)
- 3.04, 3.10, 3.02 (activated sludge, algae, golden orfe, Freitag et al. 1982)
- 2.54 (mussel *Mytilus edulis*, Geyer et al. 1982)
- 3.69 (calculated- K_{OW} , Mackay 1982)
- 4.20 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.60 (killifish, Trujillo et al. 1982)
- 1.86, 1.72, 1.60 (low-PCP flowing, high-PCP flowing, high-PCP static soft water; Brockway et al. 1984)
- 1.66, 1.62, 1.26 (low-PCP flowing, high-PCP flowing, high-PCP static hard water; Brockway et al. 1984)
- 3.10 (*alga Chlorella fusca* in culture flasks, Geyer et al. 1984; quoted, Brockway et al. 1984)
- 3.10, 2.72 (algae: exptl, calculated- K_{OW} , Geyer et al. 1984)
- 3.10, 3.02, 3.04 (algae, fish, sludge, Klein et al. 1984)
- 3.00 (quoted, LeBlanc 1984)
- 3.04, 3.10, 2.42 (activated sludge, algae, golden ide, Freitag et al. 1985)
- 0.57 (human fat, Geyer et al. 1987)
- 2.99 (zebrafish, Butte et al. 1987; quoted, Devillers et al. 1996)
- 0.46 (15°C, initial concn. 1.0 mg/L uptake by *allolobophora caliginosa* at 24 h, Haque & Ebing 1988)
- 0.38 (15°C, initial concn. 10.0 mg/L uptake by *allolobophora caliginosa* at 24 h, Haque & Ebing 1988)
- 0.80 (whole *allolobophora caliginosa*/soil, uptake from soil after 131 d exposure in outdoor lysimeters, Haque & Ebing 1988)
- 1.35 (whole *lumbricus terrestris*/soil, uptake from soil after 131 d exposure in outdoor lysimeters, Haque & Ebing 1988)
- 2.89 (quoted, Isnard & Lambert 1988)
- 2.80, 2.63 (earthworm *e. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
- 2.80, 2.63 (earthworm *e. fetida andrei*: in Kooyenburg soil, Holten soil, van Gestel & Ma 1988)
- 2.66 (daily intake/cow adipose tissue, Travis & Arms 1988; quoted, Hattemer-Frey & Travis 1989)
- 4.38, 4.50, 4.53, 4.90 (earthworm system, collated from literature, Connell & Markwell 1990)
- 4.00, 5.30, 3.40, 8.00 (earthworm system, derived data, Connell & Markwell 1990)
- 2.97, 2.11 (*p. hoyi*, *m. relict*a, Landrum & Dupuis 1990)
- 2.16–2.53 (soft tissue of freshwater mussel, Mäkelä & Oikari 1990)
- 2.33; 3.21 (flagfish: whole fish; fish lipid, Smith et al. 1990)
- 2.78, 2.11, 1.72 (goldfish at pH 7, pH 8, pH 9, Stehly & Hayton 1990)
- 3.0, 3.4, 3.9, 4.0 (perch bile to water, Söderström et al. 1994)
- 2.33; 2.58; 2.89; 2.99; 3.23 (quoted: *Jordanella floridae*; *Oryzias latipes*; *Pimephales promelas*, *Brachydanio rerio*; *Oryzias latipes*; Devillers et al. 1996)
- 3.10 (algae *Chlorella fusca*, wet wt basis, Wang et al. 1996)
- 1.41–1.59, 1.58, 2.01–2.28 (eggshell, yolk sac, embryo of lake salmon *Salmo salar* m. *sebago*, calculated- C_B/C_W , Mäenpää et al. 2004)

Sorption Partition Coefficient, log K_{OC} :

- 2.95 (soil, calculated- K_{OW} , Kenaga & Goring 1980)
- 4.72 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

- 3.11–5.65 (soil, calculated- K_{OW} , model of Karickhoff et al. 1979, Sabljic 1987a,b)
 3.17–4.54 (soil, calculated- K_{OW} , model of Kenaga & Goring 1980, Sabljic 1987a,b)
 3.37–3.69 (soil, calculated- K_{OW} , model of Briggs 1981, Sabljic 1987a,b)
 3.00–5.54 (soil, calculated- K_{OW} , model of Means et al. 1982, Sabljic 1987a,b)
 2.21–4.49 (soil, calculated- K_{OW} , model of Chiou et al. 1983, Sabljic 1987a,b)
 4.52 (sediment, Schellenberg et al. 1984; quoted, Baker et al. 2000)
 3.73 (quoted average of Kenaga & Goring 1980 & Schellenberg et al. 1984 values, Sabljic 1987a,b)
 3.46 (soil, calculated-MCI χ , Sabljic 1987a,b)
 2.95 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
 4.04 (estimated, HPLC- k' , mobile phase buffered to pH 3, Hodson & Williams 1988)
 4.40 (calculated, Lagas 1988)
 3.10, 3.26 (totally dissociated as phenolate-calculated, Lagas 1988)
 5.27, 5.71 (Bluepoint soil at pH 7.8, pH 7.4, Bellin et al. 1990)
 5.58, 5.52 (Glendale soil at pH 7.3, pH 4.3, Bellin et al. 1990)
 3.49, 3.57 (Norfolk soil at pH 4.3, pH 4.4, Bellin et al. 1990)
 4.32–4.65 (Norfolk + lime soil at pH 6.9, Bellin et al. 1990)
 4.51, 4.54 (neutral form, silt-clay slurries, Jafvert & Weber 1991)
 3.06 (calculated- K_{OW} , Kollig 1993)
 3.73 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 2.67; 3.53 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 3.67, 3.45 (pH 5, 6.5, humic acid from sediments of River Arno, De Paolis & Kukkonen 1997)
 3.64, 3.02 (pH 5, 6.5, HA + FA extracted from sediments of River Arno, De Paolis & Kukkonen 1997)
 3.90, 3.53, 3.29 (pH 5, 6.5, 8, HA extracted from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)
 3.51, 3.26 (pH 5, 6.5, 8, HA + FA from sediments of Tyrrhenian Sea, De Paolis & Kukkonen 1997)
 3.15 (pH 5, HA extracted from water of River Arno, De Paolis & Kukkonen 1997)
 3.40 (pH 5, HA + FA extracted from water of River Arno, De Paolis & Kukkonen 1997)
 3.28, 3.28, 3.15 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 2.0–> 10, average, Delle Site 2001)
 3.38, 3.51, 2.92 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH 3.4–6.9, average, Delle Site 2001)
 4.48, 4.54, 4.38 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH ≤ 3 undissociated, average, Delle Site 2001)
 2.82, 2.89, 2.63 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, $0.1 \leq OC < 0.5\%$, and pH –7.1 dissociated, average, Delle Site 2001)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization/evaporation: $t_{1/2} = 84$ h from the rate of loss experiment on watch glass for an exposure period of 192 h (Dobbs & Grant 1980);
 stripping loss rate constant $k = 0.0076$ d⁻¹ (Moos et al. 1983);
 $k = 0.028$ d⁻¹ for nondissociated PCP, assuming diffusion coefficient in air to be 7×10^{-6} m²/s and in water 7×10^{-10} m²/s with wind speed 0.1 m above the pond is 2 m/s and the average temperature is 15°C for water depth of 1 m (Crossland & Wolff 1985);
 $k(\text{calc}) = 5 \times 10^{-4}$ d⁻¹ to 1×10^{-7} d⁻¹ for total PCP (Crossland & Wolff 1985).
 Photolysis: photolysis: $t_{1/2}(\text{calc}) = 4.75$ h from observed rate $k = 3.4 \times 10^{-4}$ s⁻¹ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm² between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);
 photolysis $t_{1/2} = 1.5$ d was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);
 exposure of aqueous PCP solutions to either sunlight or laboratory ultraviolet light resulted in rapid degradation at pH 7.3 and slower degradation at pH 3.3 (Wong & Crosby 1981);
 photolytic $t_{1/2} = 10$ –15 d (Brockway et al. 1984); $k = 0.23$ to 0.46 d⁻¹ for direct photo-transformation, is the main loss process for PCP from ponds, with $t_{1/2} = 1.5$ to 3.0 d (Crossland & Wolff 1985);
 photo-transformation rate constants $k = 0.6$ h⁻¹ with $t_{1/2} = 1$ h for distilled water in summer (mean temperature 25°C) and $k = 0.37$ h⁻¹ with $t_{1/2} = 2$ h in winter (mean temperature 11°C); $k = 0.37$ h⁻¹ with $t_{1/2} = 2$ h for

- both poisoned estuarine water and estuarine water in summer and $k = 0.27 \text{ h}^{-1}$ with $t_{1/2} = 3 \text{ h}$ in winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);
- photo-mineralization rate constants $k = 0.11 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ for distilled water in summer (mean temperature 25°C) and $k = 0.049 \text{ h}^{-1}$ with $t_{1/2} = 14 \text{ d}$ in winter (mean temperature 11°C); $k = 0.12 \text{ h}^{-1}$ with $t_{1/2} = 6 \text{ d}$ for poisoned estuarine water in summer and $t_{1/2} = 0.07 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ in winter; $k = 0.25 \text{ h}^{-1}$ with $t_{1/2} = 10 \text{ d}$ for estuarine water in summer and $k = 0.10 \text{ h}^{-1}$ with $t_{1/2} = 7 \text{ d}$ for winter during days when exposed to full sunlight and microbes (Hwang et al. 1986);
- photochemical transformation $t_{1/2} = 0.75 \text{ h}$ in Xenotest 1200 (Svenson & Björndal 1988);
- aqueous $t_{1/2} = 1\text{--}110 \text{ h}$ (Hwang et al. 1986; Sugiura et al. 1984; selected, Howard et al. 1991)
- $t_{1/2} = 7.43 \text{ d}$, assuming a linear rate of photolysis during 96-h period, (Smith et al. 1987)
- photodegradation $k = 0.60 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 1.0 \text{ h}$ (summer), $k = 0.37 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 2 \text{ h}$ (winter) in distilled water; and $t_{1/2} = 0.37 \text{ h}^{-1}$ corresponding to a $t_{1/2} = 2 \text{ h}$ (summer), 0.27 h^{-1} corresponding to a $t_{1/2} = 3.0 \text{ h}$ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).
- Oxidation: aqueous oxidation rate constant $k < 7 \times 10^3 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);
- $k \gg 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ with 3 mM AcOH as scavenger for the reaction with ozone in water at pH 2.0 (Hoigné & Bader 1983b);
- photooxidation $t_{1/2} = 66\text{--}3480 \text{ h}$ in water, based on reported reaction rate constants for reaction of OH and RO_2 radicals with phenol class in aqueous solution (Mill & Mabey 1985; Güesten et al. 1981; quoted, Howard et al. 1991);
- photooxidation $t_{1/2} = 139.2\text{--}1392 \text{ h}$, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);
- rate constant $k = 4.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in air (Bunce et al. 1991)
- rate constant $k = (0.2 \pm 5.5) \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen in aqueous phosphate buffer at $27 \pm 1^\circ\text{C}$ (Tratnyek & Hoigné 1991);
- atmospheric $t_{1/2} < 24 \text{ h}$ at noon in mid-summer to $t_{1/2} = 216 \text{ h}$ in January at latitude of 41.79°N for reaction with OH radical (Bunce et al. 1991).
- Hydrolysis: is not expected to occur (Crossland & Wolff 1985).
- Biodegradation: first order microbial degradation rate constant $k = 7.4 \times 10^{-4} \text{ h}^{-1}$ in sediment and water (Yoshida & Kojima 1978, quoted, Addison et al. 1983);
- $t_{1/2} = 1800\text{--}2160 \text{ h}$ and $480\text{--}\infty \text{ h}$ to obtain 75% degradation in mineral medium and seawater, respectively (de Kreuk & Hanstveit 1981);
- $k = 0.10 \text{ d}^{-1}$ with a $t_{1/2} = 7 \text{ d}$ in unadapted Nutrient Broth and $k = 1.0 \text{ d}^{-1}$ with a $t_{1/2} = 0.7 \text{ d}$ in adapted Nutrient Broth under aerobic conditions (Mills et al. 1982);
- aqueous aerobic $t_{1/2} = 552\text{--}4272 \text{ h}$, based on unacclimated and acclimated aerobic sediment grab sample data (Delaune et al. 1983; Baker & Mayfield 1980; quoted, Howard et al. 1991);
- aqueous anaerobic $t_{1/2} = 1008\text{--}36480 \text{ h}$, based on unacclimated anaerobic grab sample data for soil and ground water (Ide et al. 1972; Baker & Mayfield 1980; quoted, Howard et al. 1991);
- aerobic degradation rate constant $k = 0.0017 \text{ L } \mu\text{g}^{-1} \cdot \text{d}^{-1}$ (Moos et al. 1983);
- microbial degradation negligible in darkness (Hwang et al. 1986);
- 100% reduction in concn ($2 \mu\text{M}$) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)
- degradation rate constant $k = 0.12 \pm 0.01 \text{ h}^{-1}$ in the absence of light (Minero et al. 1993).
- $t_{1/2}(\text{aerobic}) = 23 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 42 \text{ d}$ in natural waters (Capel & Larson 1995)
- Biotransformation: first order fish metabolism $k = 1.5 \times 10^{-5} \text{ h}^{-1}$ (Sanborn et al. 1975, quoted, Addison et al. 1983);
- bacterial transformation $k = 3 \times 10^9 \text{ mL cell}^{-1} \text{ h}^{-1}$ in water (Mabey et al. 1982);
- degradation rate $k = 3 \times 10^{-14} \text{ mol cell}^{-1} \text{ h}^{-1}$ with microorganisms in Seneca River waters (Banerjee et al. 1984).
- Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:
- $k_1 = 18.3 \text{ h}^{-1}$, 19 h^{-1} (at 1 mM buffer concn.), 18.5 h^{-1} (at 10 mM buffer concn.) at pH 8 (guppy *p. reticulata*, Saarikoski et al. 1986)
- $k_1 = 222 \text{ d}^{-1}$, 1677 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)
- $k_2 = 1.03 \text{ d}^{-1}$, 1.03 d^{-1} (flagfish: whole fish; fish lipid, Smith et al. 1990)

$k_2 = 1.03 \text{ d}^{-1}$, 0.95 d^{-1} (flagfish: BCF based, toxicity based, Smith et al. 1990)
 $k_2 = 0.00195 \pm 0.00063 \text{ h}^{-1}$ (*m. relictus*, Landrum & Dupuis 1990)
 $k_2 = 0.00330 \pm 0.00140 \text{ h}^{-1}$ (*p. hoyi*, Landrum & Dupuis 1990)
 $k_1 = 662.4 \text{ d}^{-1}$, $k_2 = 0.502 \text{ d}^{-1}$ (algae *Chlorella fusca*, Wang et al. 1996)
 $k_1 = 0.733 \text{ d}^{-1}$, $k_2 = 0.020 \text{ d}^{-1}$ (eggshell of dissected parts of lake salmon, Mäenpää et al. 2004)
 $k_1 = 0.680 \text{ d}^{-1}$, $k_2 = 0.000 \text{ d}^{-1}$ (yolk sac of dissected parts of lake salmon, Mäenpää et al. 2004)
 $k_1 = 2.828 \text{ d}^{-1}$, $k_2 = 0.015 \text{ d}^{-1}$ (embryo of dissected parts of lake salmon, Mäenpää et al. 2004)

Half-Lives in the Environment:

- Air: tropospheric lifetime of 4 d for reaction with OH radical on March 21 at 43°N (Bunce et al. 1991);
 $t_{1/2} = 139.2\text{--}1392 \text{ h}$, based on an estimated rate constant for the vapor phase reaction with hydroxyl radicals in air; photolysis $t_{1/2} = 6.5 \text{ h}$ in noonday summer sunshine (Howard 1991);
 atmospheric transformation lifetime was estimated to be $> 5 \text{ d}$ (Kelly et al. 1994).
- Surface water: calculated photolysis $t_{1/2} = 4.75 \text{ h}$ from a determined rate $k = 3.4 \times 10^{-4} \text{ s}^{-1}$ for a depth of 300 cm at pH 7 with light intensity of 0.04 watts/cm² between 290 and 330 nm on a midsummer day at the latitude of Cleveland, Ohio (Hiatt et al. 1960; quoted, Callahan et al. 1979);
 photolysis $t_{1/2} = 1.5 \text{ d}$ was estimated from photolytic destruction by sunlight in an aqueous solution at Davis, California (Wong & Crosby 1978; quoted, Callahan et al. 1979);
 photolytic $t_{1/2} = 10\text{--}15 \text{ d}$ (Brockway et al. 1984);
 rate constant $k \gg 3.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with ozone at pH 2.0 (Hoigné & Bader 1983);
 estimated direct photolysis midday $t_{1/2} = 20 \text{ min}$ from experimentally determined rate constant $k = 2.1 \text{ h}^{-1}$ (quoted unpublished result, Zepp et al. 1984);
 $t_{1/2} = 1.5 \text{ to } 3.0 \text{ d}$ for direct photo-transformation from outdoor ponds (Crossland & Wolff 1985);
 $t_{1/2} = 1 \text{ h}$ (summer), $t_{1/2} = 2 \text{ h}$ (winter) for distilled water; $t_{1/2} = 2 \text{ h}$ (summer), $t_{1/2} = 3 \text{ h}$ (winter) for estuarine water; $t_{1/2} = 2 \text{ h}$ (summer), $t_{1/2} = 3 \text{ h}$ (winter) for poisoned estuarine water, based on photo-transformation rate constants (Hwang et al. 1986); $t_{1/2} = 6 \text{ d}$ (summer), $t_{1/2} = 14 \text{ d}$ (winter) for distilled water; $t_{1/2} = 3 \text{ d}$ (summer), $t_{1/2} = 7 \text{ d}$ (winter) for estuarine water; $t_{1/2} = 6 \text{ d}$ (summer), $t_{1/2} = 10 \text{ d}$ (winter) for poisoned estuarine water, based on photo-mineralization rate constants (Hwang et al. 1986);
 $t_{1/2} = 0.75 \text{ h}$ and 0.96 h , based on photochemical transformation in Xenotest 1200 (Svenson & Björndal 1988);
 $t_{1/2} = 1\text{--}110 \text{ h}$, based on aqueous photolysis half-life (Howard et al. 1991);
 photodegradation half-lives ranging from hours to days, more rapid at the surface (Howard 1991);
 photodegradation $t_{1/2} = 1.0 \text{ h}$ (summer), $t_{1/2} = 2.0 \text{ h}$ (winter) in distilled water and $t_{1/2} = 2.0 \text{ h}$ (summer), $t_{1/2} = 3.0 \text{ h}$ (winter) in estuarine water under irradiation by natural sunlight (quoted from Hwang et al. 1987, Sanders et al. 1993).
 $t_{1/2}(\text{aerobic}) = 23 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 42 \text{ d}$ in natural waters (Capel & Larson 1995)
- Ground water: $t_{1/2} = 1104\text{--}36480 \text{ h}$, based on estimated unacclimated aqueous aerobic sediment grab sample data (Delaune et al. 1983; selected, Howard et al. 1991) and unacclimated anaerobic grab sample data for ground water (Baker & Mayfield 1980; selected, Howard et al. 1991).
- Sediment: first order microbial degradation rate constant $k = 7.4 \times 10^{-4} \text{ h}^{-1}$ in sediment and water (Yoshida & Kojima 1978, quoted, Addison et al. 1983).
- Soil: Days for complete disappearance by microbial decomposition in soil suspension: $72 + \text{d}$ in Dunkirk silt loam (Alexander & Aleem 1961)
 disappearance $t_{1/2} = 23.2 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 47.9 \text{ d}$ from Holten soil with earthworm *e. fetida andrei* and $t_{1/2} = 27.4 \text{ d}$ from Kooyenburg soil, $t_{1/2} = 31.8 \text{ d}$ from Holten soil with earthworm *I. rubellus* (van Gestel & Ma 1988);
 $t_{1/2} = 552\text{--}4272 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);
 $t_{1/2} = 2.0 \text{ d}$ in an acidic clay soil with $< 1.0\%$ organic matter and $t_{1/2} = 6.7 \text{ d}$ in a slightly basic sandy loam soil with 3.25% organic matter, based on aerobic batch lab microcosm experiments (Loehr & Matthews 1992).
- Biota: biological $t_{1/2} = 30 \text{ d}$ in guppy *lebistes reticulatus* (Landner et al. 1977);
 elimination $t_{1/2} = 23, 9.3, 6.9$, and 6.2 h for fat, liver muscle, and blood, respectively (rainbow trout, Call et al. 1980);
 estimated $t_{1/2} = 7.0 \text{ d}$ in trout (Niimi & Cho 1983; quoted, Niimi & Palazzo 1985);
 clearance from flagfish: $t_{1/2} = 0.68 \text{ d}$ from whole fish and $t_{1/2} = 0.68 \text{ d}$ from fish lipid (Smith et al. 1990).

TABLE 14.1.2.13.1
Reported aqueous solubilities of pentachlorophenol at various temperatures

Carswell & Nason 1938		Achard et al. 1996		Jaoui et al. 1999	
shake flask		shake flask-conductivity		static visual method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	T/K	S/g·m ⁻³
0	5	25.1	21.4	333.2	102
27	18	34.5	57.8	342.7	118.4
50	35	46.8	86.2	353.2	140.6
62	58			361.2	156.8
70	85			372.0	173.1
				386.0	195.3
				402.0	211.6
				407.0	232.3
				422.3	253.0

Note: PCP data in Table I
incorrect, correction made
Figure 3 in ref
based on Figure 3 in ref.

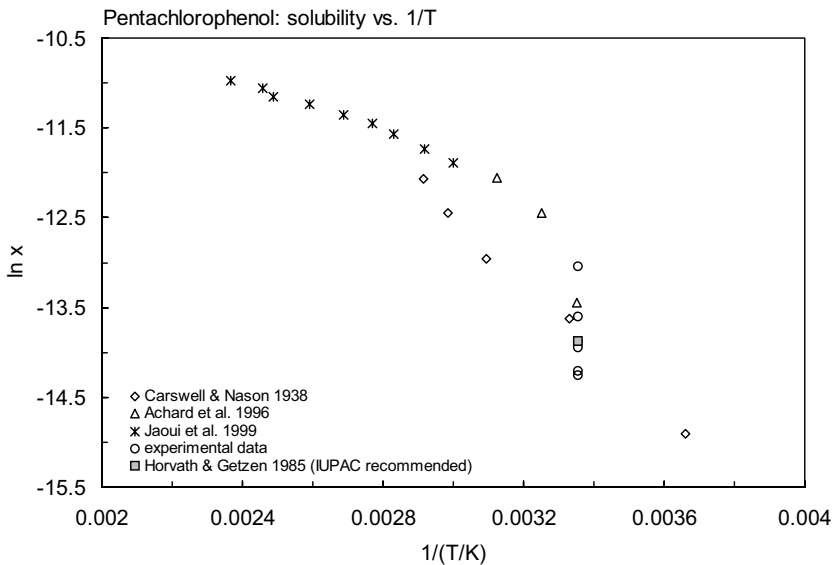


FIGURE 14.1.2.13.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for pentachlorophenol.

TABLE 14.1.2.13.2

Reported vapor pressures of pentachlorophenol at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)				
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)				
$\log P = A - B/(C + T/K)$	(3)						
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)						
Carswell & Nason 1938	Stull 1947	McDonald et al. 1959	Rordorf 1989				
static method	summary of literature data	ebulliometry	gas saturation-GC				
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
0	0.00227*	192.2	2666	46.0	0.108	25	0.0070
20	0.0227*	211.2	5333	60.0	0.1853	50	0.110
50	0.4133*	223.4	7999	70.0	0.2573	75	1.20
75	3.200*	239.6	13332	71.8	0.3960	100	9.50
100	18.67	261.8	26664	80.0	0.9746	125	57.0
120	63.99	285.0	53329	93.6	3.3597		
140	200.0	309.3	101325	106.5	8.5460		for solid
160	573.3			119.5	23.60	eq. 1	P _s /Pa
180	1453	mp/°C	188.5	200.6	4133	A	13.413
200	3413			215.51	6759	B	4640.9
220	7493			233.87	12279		
240	14705*						for liquid
260	30358*			eq. 2	P/mmHg	eq. 1	P _L /Pa
280	56622*			A	9.073	A	11.47085
300	101112*			B	3606.0	B	3750.68
300.6	101325			C	273.15		
measured range 100–220°C				mp/°C	189.65		
*extrapolated from graph							

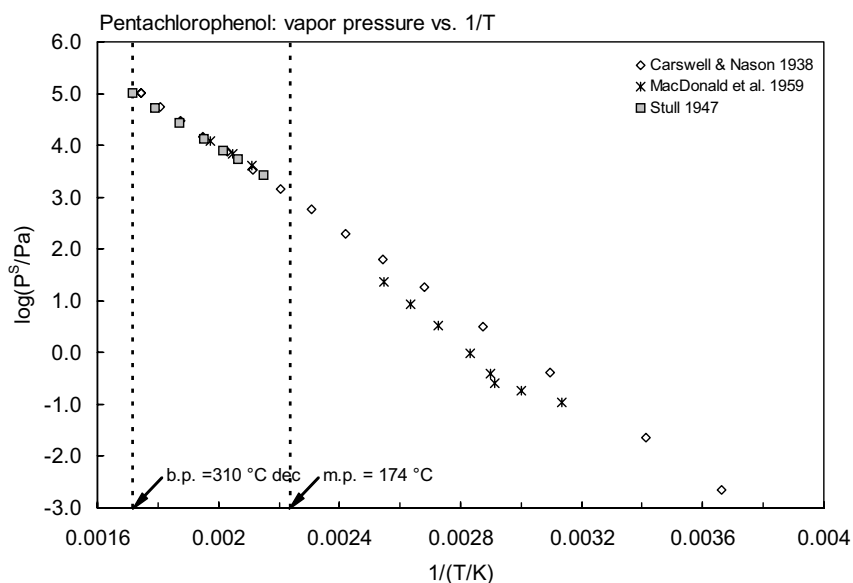
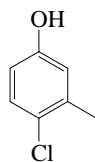


FIGURE 14.1.2.13.2 Logarithm of vapor pressure versus reciprocal temperature for pentachlorophenol.

14.1.2.14 4-Chloro-*m*-cresol

Common Name: 4-Chloro-*m*-cresol

Synonym: *p*-chloro-*m*-cresol, 2-chloro-5-hydroxytoluene, 4-chloro-3-methylphenol

Chemical Name: 4-chloro-*m*-cresol, 4-chloro-3-methylphenol

CAS Registry No: 59-50-7

Molecular Formula: C_7H_7ClO , $CH_3(Cl)C_6H_3OH$

Molecular Weight: 142.583

Melting Point ($^{\circ}C$):

67 (Lide 2003)

Boiling Point ($^{\circ}C$):

235.0 (Weast 1977; Callahan et al. 1979; Dean 1985; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

146.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, $F: 0.387$ (mp at $67^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

3990 (shake flask-UV with buffer at pH 5.1, Blackman et al. 1955)

3990 (IUPAC selected, Horvath & Getzen 1985)

3650 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

6.67 (Mabey et al. 1982)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.253 ($20^{\circ}C$, calculated-P/C, Mabey et al. 1982)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.18 (Hansch & Leo 1979)

2.95 (calculated as per Tute 1971, Callahan et al. 1979)

3.10 (HPLC-RT correlation, Veith et al. 1979)

3.10 (recommended, Sangster 1993)

3.10 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

2.60 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{oc}$:

2.78 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

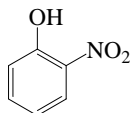
Oxidation: rate constants $k < 7 \times 10^5 M^{-1} h^{-1}$ for singlet oxygen and $k = 1 \times 10^7 M^{-1} h^{-1}$ for peroxy radical (Mabey et al. 1982).

Biotransformation: bacterial transformation $k = 3 \times 10^{-9} mL cell^{-1} h^{-1}$ in water (Mabey et al. 1982).

Half-Lives in the Environment:

14.1.3 NITROPHENOLS

14.1.3.1 2-Nitrophenol



Common Name: 2-Nitrophenol

Synonym: *o*-nitrophenol, 2-hydroxynitrobenzene

Chemical Name: 2-nitrophenol

CAS Registry No: 88-75-5

Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$

Molecular Weight: 139.109

Melting Point (°C):

44.8 (Lide 2003)

Boiling Point (°C):

216.0 (Weast 1982-83; Lide 2003)

Density (g/cm³ at 20°C):

1.485, 1.2942 (14, 40°C, Weast 1982-83)

131.9 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

7.21 (Pearce & Simkins 1968)

7.23 (Serjeant & Dempsey 1979)

8.28 (Mabey et al. 1982)

7.22 (Dean 1985)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

17.57 (Tsonopoulos & Prausnitz 1971)

17.44 (Beneš & Dohnal 1999)

Entropy of Fusion, ΔS_{fus} (J/mol K):

55.23 (Tsonopoulos & Prausnitz 1971)

48.95, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at 25°C (assuming $\Delta S_{fus} = 56$ J/mol K), F : 0.630 (mp at 44.8°C)

Water Solubility (g/m³ or mg/L at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

3210* (38.4°C, shake flask-residue volume method, measured range 34.8–196°C, critical solution temp above 200°C, Sidgwick et al. 1915)

1390, 1095 (20°C, shake flask-UV, calculated, Hashimoto et al. 1984)

1080* (20 ± 0.5°C, shake flask-UV with buffer at pH 1.5, measured range 5–30°C, Schwarzenbach et al. 1985)

2100 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

1697* (24.8°C, shake flask-conductimetry, measured range 15.6–34.7°C, Achard et al. 1996)

1350* (20°C, shake flask-UV spectrophotometry, measured range 10–40°C, Beneš & Dohnal 1999)

1169* (17.35°C, shake flask-optical method, measured range 290.5–322.7 K, Jaoui et al. 2002)

$\ln [S/(\text{mol kg}^{-1})] = 16.237 - 4672.3/(T/K)$; temp range 288–308 K (eq. derived using reported exptl. data, Jaoui et al. 2002)

$\ln [S/(\text{mol kg}^{-1})] = 6.9022 - 1784.4/(T/K)$; temp range 308–332 K (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29.10* (extrapolated-regression of tabulated data, temp range 49.3–214.5°C, Stull 1947)

$\log (P/\text{mmHg}) = [-0.2185 \times 12497.3/(T/K)] + 8.497320$; temp range 49.3–214.5°C (Antoine eq., Weast 1972–73)

- 24.43 (extrapolated-Cox eq., Chao et al. 1983)
 $\log (P/\text{mmHg}) = [1 - 487.905/(T/K)] \times 10^4 \{0.885400 - 6.30106 \times 10^{-4} \cdot (T/K) + 6.42867 \times 10^{-7} \cdot (T/K)^2\}$; temp range: 322.5–487.7 K (Cox eq., Chao et al. 1983)
 12.4 \pm 0.2 (gas saturation-HPLC/UV, Sonnefeld et al. 1983)
 17.25 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)
 $\log (P_s/\text{kPa}) = 7.8446 - 2864.6/(T/K)$, temp range 273–292 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.04963 - 1571.7/(-101.17 + T/K)$, temp range 366–490 K (liquid, Antoine eq.-II, Stephenson & Malanowski 1987)
 18.86 (supercooled liquid P_L at 20°C, GC-RT correlation, Schwarzenbach et al. 1988)
 10.61 (20°C, solid P_s , converted from P_L with ΔS_{fus} and mp, Schwarzenbach et al. 1988)
 $\log (P/\text{atm}) = 5.735 - 2776/(T/K)$ (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 0.766 (calculated-P/C, Mabey et al. 1982)
 0.355 (Leuenberger et al. 1985)
 1.367 (20°C, calculated-P/C, Schwarzenbach et al. 1988)
 1.25* (gas stripping-UV, measured range 5–40°C, Müller & Heal 2001)
 $\ln [H/(M \text{ atm}^{-1})] = 6290/(T/K) - 16.6$; temp range 278–303 K (gas stripping-UV, Müller & Heal 2001)
 1.178* (gas stripping-UV, measured range 284–302 K, Harrison et al. 2002)
 $\ln [H/(M \text{ atm}^{-1})] = 6270/(T/K) - 16.6$; temp range 284–302 K, Harrison et al. 2002)

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

- 1.79 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971)
 2.00 (shake flask, Umeyama et al. 1971)
 1.25, 1.18 (calculated-fragment const., calculated- π const., Rekker 1977)
 1.79 (shake flask, Korenman et al. 1977)
 1.68 (shake flask at pH 7, Unger et al. 1978)
 1.35 (HPLC-RT correlation, Veith et al. 1979)
 1.91 (HPLC-RT correlation, Miyake et al. 1986)
 1.89 ($21.5 \pm 0.5^\circ\text{C}$, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)
 1.76 (shake flask-UV, Kramer & Henze 1990)
 1.68 (CPC-RV at pH 7.4, El Tayar et al. 1991)
 2.24 (HPLC-RT correlation, Saito et al. 1993)
 1.77 (recommended, Sangster 1993)
 1.85, 1.79 (COMPUTOX databank, Kaiser 1993)
 1.79, 1.68 (recommended, value at pH 7.4; Hansch et al. 1995)
 2.03 (solid-phase microextraction, Dean et al. 1996)
 1.63, 1.99, 2.28, 1.90 (HPLC- k' correlation, different combinations of stationary and mobile phases under isocratic conditions, Makovskaya et al. 1995a)

Bioconcentration Factor, $\log \text{BCF}$:

- 2.10 (bluegill sunfish, Veith et al. 1980)
 1.23 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)
 1.15 (calculated- K_{ow} , Howard 1989)

Sorption Partition Coefficient, $\log K_{\text{oc}}$:

- 1.43 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)
 1.81 (soil, calculated-S, quoted, Howard 1989)
 2.17; 2.50 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 2.424, 1.507, 1.852, 1.763, 2.336 (first generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1998, 1999)
 2.043, 1.758, 1.854, 1.708, 2.283 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV, Gawlik et al. 1999)

2.043, 1.758, 1.854, 1.708, 2.283 (second generation Eurosoils ES-1, ES-2, ES-3, ES-4, ES-5, shake flask/batch equilibrium-HPLC/UV and HPLC- k' correlation, Gawlik et al. 2000)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} = 296$ h from a model river was estimated using Henry's law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind (Howard 1989)

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

rate constant $k < 2 \times 10^5 \text{ M}^{-1}\cdot\text{h}^{-1}$ for singlet oxygen, and $k = 2 \times 10^6 \text{ M}^{-1}\cdot\text{h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);

$k_{OH} = 0.922 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ at 296 K (Becker et al. 1984; quoted, Carlier et al. 1986);

$k_{OH}(\text{exptl}) = 0.92 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1985)

$k_{OH}(\text{exptl}) = 0.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{calc}) = 4.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1987)

$k_{OH} = 0.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 294 K (Atkinson 1989)

photooxidation $t_{1/2} = 7\text{--}71$ h, based on measured rate data for the vapor phase reaction with OH radical in air (Howard et al. 1991)

$k_{O_3} = 2.0 \times 10^{-23} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 298 K, measured range 298–323 K (quoted, Atkinson & Carter 1984)

$k_{OH} = (2.34 \pm 0.33) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $(24.6 \pm 0.4)^\circ\text{C}$ (Edney et al. 1986)

$k_{OH} = 2.34 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 298 K, $k_{NO_3} = 9.7 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Atkinson 1990)

$k_{NO_3} < 0.02 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1} \text{ s}^{-1}$ at 296 K and $k_{OH} = 0.90 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (Atkinson 1991)

aqueous photooxidation $t_{1/2} = 480$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992)

photo-transformation decay rate constant $k = 0.27 \text{ min}^{-1}$ on 0.2 g/L of TiO_2 solution (Minero et al. 1993).

Hydrolysis: resistant to hydrolysis (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $14.0 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mg/L in 3–5 d by wastewater and 7–14 d by soil (Haller 1978);

aqueous aerobic $t_{1/2} = 168\text{--}672$ h, based on unacclimated aerobic screening test data (Sasaki 1978; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 168\text{--}672$ h, based on anaerobic soil grab sample data (Sudhakar-Barik & Sethunathan 1978; selected, Howard et al. 1991).

Biotransformation: estimated bacterial transformation rate constant of $2 \times 10^{-9} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 14$ h for the gas phase reaction with hydroxyl radical (GEMS 1986; quoted, Howard 1989)

photooxidation $t_{1/2} = 7\text{--}71$ h, based on measured rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991).

Surface water: $t_{1/2} = 168\text{--}672$ h, based on aerobic river die-away test data (Ludzack et al. 1958; selected value, Howard et al. 1991);

volatilization $t_{1/2} = 12$ d from a model river was estimated using Henry's law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind and $t_{1/2} = 1\text{--}8$ d in freshwater (Howard 1989);

calculated $t_{1/2} = 390$ h for a body of water with 1 m in depth (Schmidt-Bleek et al. 1982; quoted, Howard 1989);

photooxidation $t_{1/2} = 480$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Groundwater: $t_{1/2} = 336\text{--}672$ h, based on estimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 10$ d in flooded soil (Howard 1989);

$t_{1/2}$ = 168–672 h, based on estimated aqueous aerobic biodegradation half-life and anaerobic soil grab sample data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991).

Biota:

TABLE 14.1.3.1.1

Reported aqueous solubilities of 2-nitrophenol at various temperatures

Sidgwick et al. 1915		Schwarzenbach et al. 1988		Beneš & Dohnal 1999		Jaoui et al. 2002	
shake flask-synthetic method		shake flask-UV spec.		shake flask-UV spec		shake flask-optical method	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
solid							
38.4	3210	0	747	10	895	17.35	1169
42.8	3460	10	898	20	1350	31.35	2434
47.5	3760	20	1080	30	2000	36.85	3144
59.4	4550	30	1457	40	2840	49.55	3951
65.7	5130	for supercooled liquid			17.35	1169	
72.8	5890	0	2058	mp/K	317.95	30.05	2281
80.3	6900	10	1920	$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 17.44$		37.55	3186
88.9	8330	20	2011	Enthalpies of solution*:		49.55	3951
109.9	13430	30	1877	$\Delta H_{\text{sol}}(\text{solid}) = 28.7 \text{ kJ mol}^{-1}$		17.35	1169
151.8	30300			$\Delta H_{\text{sol}}(\text{liq.}) = 11.2 \text{ kJ mol}^{-1}$		31.25	2434
169.5	50400					36.85	3144
196.5	99000					49.55	3951
...	...	Achard et al. 1996					
196.5	906800	shake flask-conductimetry					
163.4	951400	t/°C	S/g·m ⁻³				
91.7	984800						
82.9	987300	15.6	1076				
59.3	992400	24.8	1697				
43.6	995100	34.7	2935				
44.9	1000000						
critical solution temp >200°							
triple point 43.5°C							

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

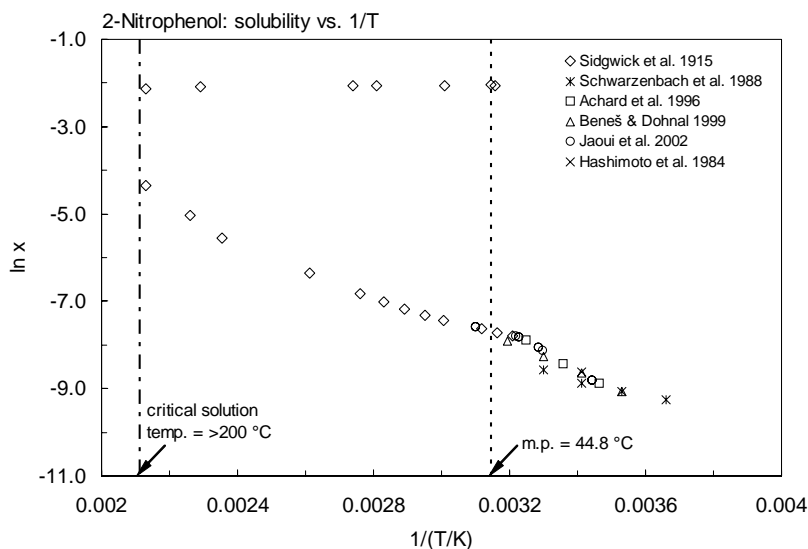


FIGURE 14.1.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2-nitrophenol.

TABLE 14.1.3.1.2

Reported vapor pressures and Henry's law constants of 2-nitrophenol at various temperatures and the coefficients for the vapor pressure equations

$$\log P = A - B/(T/K) \quad (1) \qquad \ln P = A - B/(T/K) \quad (1a)$$

$$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C}) \quad (2) \qquad \ln P = A - B/(C + t/^{\circ}\text{C}) \quad (2a)$$

$$\log (P/\text{Pa}) = A - B/(C + T/K) \quad (3)$$

$$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K) \quad (4)$$

Vapor pressure		Henry's law constant			
Stull 1947		Müller & Heal 2001		Harrison et al. 2002	
summary of literature data		gas stripping-UV spec.		gas stripping-UV	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	$H/(\text{Pa m}^3/\text{mol})$	T/K	$H/(\text{Pa m}^3/\text{mol})$
non-equilibrium					
49.3	133	5	0.274	281	0.362
76.8	666.6	10	0.442	284.5	0.396
90.4	1333	15	0.600	289.5	0.607
105.8	2666	20	0.641	293.5	0.930
122.1	5333	25	1.267	298	1.178
132.6	7999	30	1.689	302	1.559
146.4	13332	equilibrium			
167.6	26664	5	0.242	eq. 4	$H=/(M \text{ atm}^{-1})$
191.0	53329	10	0.409	A	-16.6
214.5	101325	15	0.569	B	-6270
		20	0.714		
mp/ $^{\circ}\text{C}$	45	25	1.251		
		30	1.608		
eq.4 $H=/(M \text{ atm}^{-1})$					
A -16.6					
B -6290					
For gas-to-liquid transfer					
$\Delta H^{\circ}/(\text{kJ mol}^{-1}) = -52.3 \pm 8.1$					
$\Delta S^{\circ}/(\text{J mol}^{-1}\text{K}^{-1}) = -138 \pm 28$					

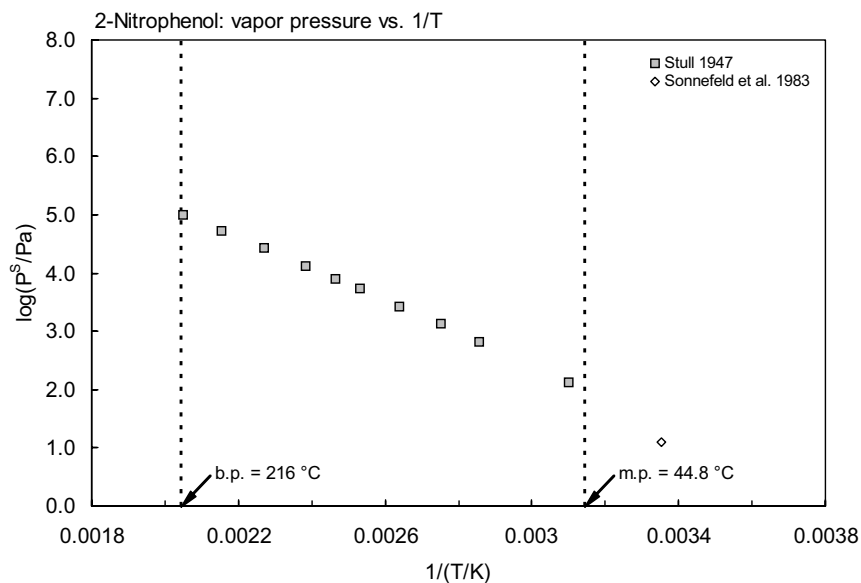


FIGURE 14.1.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for 2-nitrophenol.

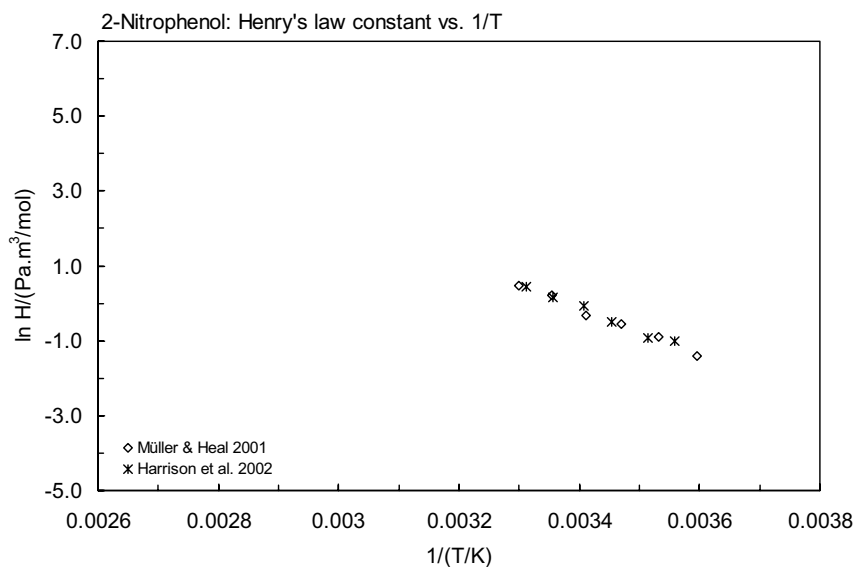
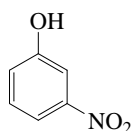


FIGURE 14.1.3.1.3 Logarithm of Henry's law constant versus reciprocal temperature for 2-nitrophenol.

14.1.3.2 3-Nitrophenol



Common Name: 3-Nitrophenol

Synonym: *m*-nitrophenol

Chemical Name: 3-nitrophenol

CAS Registry No: 554-84-7

Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$

Molecular Weight: 139.109

Melting Point ($^{\circ}C$):

96.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

194.0 (at 70 mm Hg, Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

1.2797 ($10^{\circ}C$, Verschueren 1983)

Molar Volume (cm^3/mol):

108.7 ($100^{\circ}C$, Stephenson & Malanowski 1987)

131.9 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

8.00 (Fieser & Fieser 1958)

8.36 (Serjeant & Dempsey 1979; Dean 1985; Howard 1989; Haderlein & Schwarzenbach 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.34 (Tsonopoulos & Prausnitz 1971)

19.20 (Beneš & Dohnal 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

57.74 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.197 (mp at $96.8^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

30300* ($40.4^{\circ}C$, shake flask-residue volume method, measured range 40.4 – $98.7^{\circ}C$, critical solution temp $98.7^{\circ}C$, Sidgwick et al. 1915)

13000 (shake flask-UV spectrophotometry, Roberts et al. 1977)

11546 ($20^{\circ}C$, shake flask-UV, Hashimoto et al. 1984)

10800* ($20^{\circ}C$, shake flask-UV spectrophotometry, measured range 10 – $40^{\circ}C$, Beneš & Dohnal 1999)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

3.83×10^{-2} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 8.93697 - 3981.386/(T/K)$, temp range 305 – $334\ K$ (solid, Antoine eq., Stephenson & Malanowski 1987)

99.98 (Weber et al. 1981)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2.203×10^{-4} (quoted, Gaffney et al. 1987)

1.033 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.00 (shake flask-UV, Fujita et al. 1964; Leo et al. 1971)

2.00 (shake flask-UV at pH 5.6, Umeyama et al. 1971)

2.00 ($20^{\circ}C$, shake flask, Korenman et al. 1976)

2.02	(Scherrer & Howard 1979)
1.74	(HPLC-RT correlation, Butte et al. 1981)
2.05	(Beltrame et al. 1988, 1989)
2.01, 2.03	(shake flask, HPLC-RT correlation, Wang et al. 1989)
1.88	(shake flask-UV, Kramer & Henze 1990)
1.74	(centrifugal partition chromatography CPC-RV at pH 7.4, El Tayar et al. 1991)
2.00	(recommended, Sangster 1993)
1.92, 1.51	(COMPUTOX databank, Kaiser 1993)
2.00	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.40	(goldfish, ratio of rate constant k_1/k_2 , Nagel & Urich 1980)
1.40	(<i>Brachydanio rerio</i> , Butte et al. 1987)
1.28	(estimated- K_{ow} , Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

1.72	(Brookton clay loam, Boyd 1982)
1.36	(soil, estimated-S, Howard 1989)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: volatilization $t_{1/2} = 4.2$ d from a model river was estimated using Henry's law constant for a model river of 1 m deep with 1 m/s current and a 3 m/s wind (Howard 1989).

Photolysis:

Oxidation: photooxidation $t_{1/2} \sim 14$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard 1989);

phototransformation decay rate $k = 0.18 \text{ min}^{-1}$ in 0.2 g/L of TiO_2 solution (Minero et al. 1993).

Hydrolysis: resistant to hydrolysis (Howard 1989).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

decomposition by a soil microflora in 4 d (Alexander & Lustigman 1966; quoted, Verschuereen 1983)

complete degradation of 16 mg/L in 3–5 d by wastewater, and 3–5 d by soil (Haller 1978);

average rate of biodegradation $17.5 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

$t_{1/2} = 6.3$ d or less in flooded soil under anaerobic conditions (Howard 1989)

$t_{1/2}(\text{aerobic}) = 0.76$ d, $t_{1/2}(\text{anaerobic}) = 6.8$ d in natural waters (Capel & Larson 1995).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 1.54 \text{ h}^{-1}$; $k_2 = 0.00 \text{ h}^{-1}$ (goldfish, Nagel & Urich 1980)

Half-Lives in the Environment:

Air: $t_{1/2} = 14$ h for reaction with hydroxyl radical in vapor phase (Howard 1989).

Surface water: $t_{1/2} = 4.2$ d in a model river (Howard 1989)

$t_{1/2}(\text{aerobic}) = 0.76$ d, $t_{1/2}(\text{anaerobic}) = 6.8$ d in natural waters (Capel & Larson 1995).

Groundwater:

Sediment:

Soil: $t_{1/2} = 6.3$ d in flooded soil under anaerobic conditions (Howard 1989).

Biota: elimination from goldfish within 4 h (Nagel & Urich 1980).

TABLE 14.1.3.2.1
Reported aqueous solubilities of 3-nitrophenol at various temperatures

Sidgwick et al. 1915						Beneš & Dohnal 1999	
shake flask-synthetic method						shake flask-UV spec	
t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³	t/°C	S/g·m ⁻³
40.4	30300	98.5	291000	72.7	673800	10	7200
49.5	36500	98.5	351300	55.8	715600	20	10800
61.1	46600	98.6	388400	42.3	758900	30	16700
67.1	54200	98.7	409400	43.9	793200	40	19000
79.1	76400	98.5	431200	62.0	899000		
85.1	94700	97.9	481200	95.1	1000000	mp/K	369.95
88.5	109400	94.5	539500			$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 19.20$	
93.2	139200	91.9	571900	critical solution temp 98.7°C		Enthalpies of solution*:	
97.1	188500	87.3	607400	triple point 41.5°C		$\Delta H_{\text{sol}}(\text{solid}) = 29.3 \text{ kJ mol}^{-1}$	
98.0	215500	82.6	634700			$\Delta H_{\text{sol}}(\text{liq.}) = 16.1 \text{ kJ mol}^{-1}$	

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

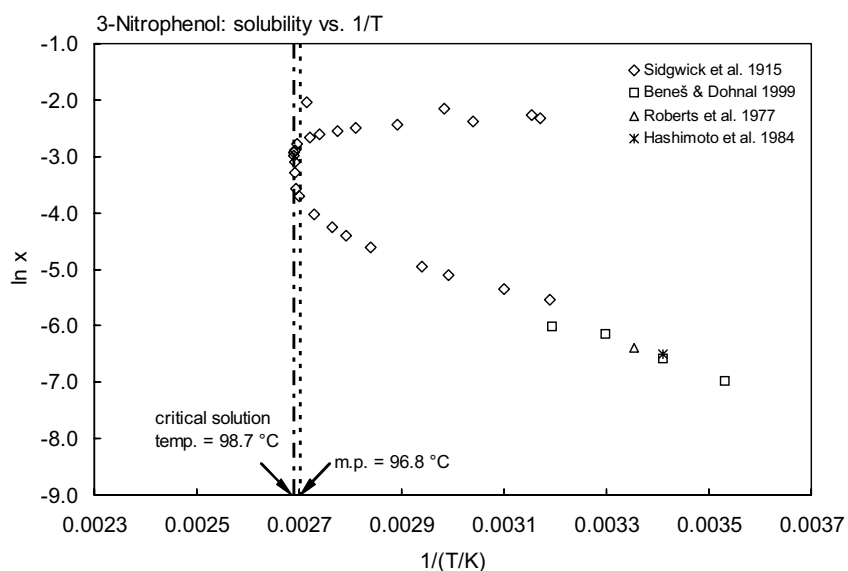
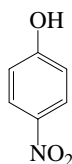


FIGURE 14.1.3.2.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 3-nitrophenol.

14.1.3.3 4-Nitrophenol



Common Name: 4-Nitrophenol

Synonym: *p*-nitrophenol, 4-hydroxynitrobenzene

Chemical Name: 4-nitrophenol

CAS Registry No: 100-02-7

Molecular Formula: $C_6H_5NO_2$, $C_6H_4(NO_2)OH$

Molecular Weight: 139.109

113.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

279.0 (decomposes, Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.479 (Weast 1982–83)

Molar Volume (cm^3/mol):

131.9 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

7.08 (21.5 $^{\circ}C$, UV, Schwarzenbach et al. 1988)

7.17 (Fieser & Fieser 1958)

7.16 (Serjeant & Dempsey 1979; Howard 1989; Haderlein & Schwarzenbach 1993)

7.15 (Dean 1985; Miyake et al. 1987; Brecken-Folse et al. 1994; Howe et al. 1994)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

15.90 (Tsonopoulos & Prausnitz 1971)

18.25 (Beneš & Dohnal 1999)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

41.09 (Tsonopoulos & Prausnitz 1971)

62.76, 56.5 (observed, estimated, Yalkowsky & Valvani 1980)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.135 (mp at $113.6^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

29100* (34.8 $^{\circ}C$, shake flask-residue volume method, measured range 34.8–92.8 $^{\circ}C$, critical solution temp 92.8 $^{\circ}C$, Sidgwick et al. 1915)

14000 (shake flask-spectrophotometry, Roberts et al. 1977)

9950, 14800 (15, 25 $^{\circ}C$, shake flask, average values of 6 laboratories, OECD 1981)

13490, 11140 (20 $^{\circ}C$, shake flask-UV, calculated, Hashimoto et al. 1984)

11570 (20 \pm 0.5 $^{\circ}C$, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)

16000 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

15599* (shake flask-conductimetry, measured range 15.3–34.9 $^{\circ}C$, Achard et al. 1996)

12200* (20 $^{\circ}C$, shake flask-UV spectrophotometry, measured range 10–38 $^{\circ}C$, Beneš & Dohnal 1999)

15052* (23.65 $^{\circ}C$, shake flask-optical method, measured range 285.9–313.8 K, Jaoui et al. 2002)

$\ln [S/(mol\ kg^{-1})] = 17.110 - 4273.4/(T/K)$; temp range 288–314 K (eq. derived using reported exptl. data, Jaoui et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0054 (20 $^{\circ}C$, Schmidt-Bleek et al. 1982)

0.0012 (selected, Yoshida et al. 1983)

0.0044 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.9529 - 5159.7/(T/K)$, temp range 304–352 K (solid, Antoine eq., Stephenson & Malanowski 1987)

- 0.111 (supercooled liquid P_L at 20°C, GC-RT correlation, Schwarzenbach et al. 1988)
 0.0131 (20°C, solid P_S , converted from P_L with ΔS_{fus} and mp, Schwarzenbach et al. 1988)
 $\log(P/\text{mmHg}) = 8.305 - 4180/(T/K)$ (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)
 0.133 (Howard 1989)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 4.21×10^{-5} (exptl., Hine & Mookerjee 1975)
 5.55×10^{-4} , 9.87×10^{-3} (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 1.04×10^{-5} (calculated-P/C, Yoshida et al. 1983)
 0.00335 (20°C, calculated-P/C, Schwarzenbach et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 1.91 (shake flask-UV, Fujita et al. 1964; quoted, Leo et al. 1971; Hansch & Leo 1979)
 1.18, 1.27 (calculated- π const., calculated-fragment const., Rekker 1977)
 1.68 ± 0.01 (RP-HPLC- k' correlation, Unger et al. 1978)
 2.07 (RP-HPLC- k' correlation, Miyake & Terada 1982)
 1.86 (HPLC-ref. substances extrapolated, Harnish et al. 1983)
 1.88 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
 1.96 ± 0.08 (HPLC-RV correlation.-ALPM, Garst 1984; Garst & Wilson 1984)
 1.85, 1.92 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)
 0.70 (calculated- γ from UNIFAC, Campbell & Luthy 1985)
 1.90 (HPLC-RV correlation, Brooke et al. 1986)
 2.10 (HPLC- k' correlation, Miyake et al. 1987)
 1.93 (shake flask/batch equilibration-UV, Beltrame et al. 1988, 1989)
 2.04 ($21.5 \pm 1.5^\circ\text{C}$, shake flask-UV with buffer at pH 1.5, Schwarzenbach et al. 1988)
 1.77 (CPC-RV at pH 7.4, El Tayar et al. 1991)
 1.85, 1.91 (COMPUTOX databank, Kaiser 1993)
 1.91 (recommended, Sangster 1993)
 1.90 ± 0.14 , 1.09 ± 0.53 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
 1.91 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log BCF$:

- 2.10 (fathead minnow, Veith et al. 1980)
 2.56 (mean whole body ^{14}C in fathead minnow, Call et al. 1980)
 1.90, 2.34 (total ^{14}C in fathead minnow: observed, calculated, mean exposure level $0.0041 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
 2.44, 2.65 (total ^{14}C in fathead minnow: observed, calculated, mean exposure level $0.0441 \mu\text{g}\cdot\text{mL}^{-1}$, Call et al. 1980)
 1.76; 1.04 (golden orfe; green algae, Freitag et al. 1982)
 1.48 (activated sludge, Freitag et al. 1982)
 1.43 (microorganisms-water, calculated- K_{ow} , Mabey et al. 1982)
 0.301 (calculated- K_{ow} , Yoshida et al. 1983)
 1.48, 1.45 (alga *Chlorella fusca*, wet wt. basis, calculated- K_{ow} , Geyer et al. 1984)
 1.60, 1.48, 1.48 (golden ide, algae, activated sludge, Freitag et al. 1985)
 1.90 (fathead minnow, quoted, Howard 1989)

Sorption Partition Coefficient, $\log K_{oc}$:

- 1.65 (sediment-water, calculated- K_{ow} , Mabey et al. 1982)
 2.41 (soil, calculated- K_{ow} , Yoshida et al. 1983)
 1.74 (Brookston clay loam, Boyd 1982)
 2.18 (HPLC- k' correlation, cyanopropyl column, mobile phase buffered to pH 3, Hodson & Williams 1988)
 1.32 (soil, calculated-S, Howard 1989)
 2.37 (soil, quoted exptl., Meylan et al. 1992)
 2.49 (soil, calculated-MCI χ and fragment contribution, Meylan et al. 1992)

- 2.16, 2.07 (RP-HPLC- k' correlation including MCI related to non-dispersive intermolecular interactions, hydrogen-bonding indicator variable, Hong et al. 1996)
 2.05; 2.49 (HPLC-screening method; calculated-PCKOC fragment method, Müller & Kördel 1998)
 2.03, 1.94 (soils: organic carbon $OC \geq 0.1\%$, $OC \geq 0.5\%$, and $pH \leq 5.4$, average, Delle Site 2001)

Environmental Fate Rate Constants, k or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: atmospheric photolysis $t_{1/2} = 3.1\text{--}329$ h, based on sunlight photolysis at pH 9 and pH 4 (Hustert et al. 1981; Lemaire et al. 1985; selected, Howard et al. 1991);
 rate constant $k = 3.96 \times 10^{-3} \text{ h}^{-1}$ for the direct photolysis in water (Yoshida et al. 1983);
 photolysis $t_{1/2}$ range from hours to a week or more in atmosphere and $t_{1/2} = 2\text{--}14$ d in clear surface waters (Howard 1989).

Oxidation: oxidation rate constant $k < 2 \times 10^5 \text{ M}^{-1}\cdot\text{h}^{-1}$ for singlet oxygen, $k = 2 \times 10^6 \text{ M}^{-1}\cdot\text{h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 21$ d to 5.6 y in water, based on rate constants for reaction in water with hydroxyl radical (Dorfman & Adams 1973; Scully & Hoigné 1987; selected, Howard et al. 1991);

rate constant $k < 50 \text{ M}^{-1}\cdot\text{s}^{-1}$ for 0.01–14 mM to react with ozone in water using PrOH as scavenger at pH 1.7 and 20–23°C in water (Hoigné & Bader 1983a,b);

rate constant $k = 8.3 \times 10^{-12} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ for the gas-phase reaction with OH radical at 296 K in the atmosphere (Becker et al. 1984; quoted, Carlier et al. 1986);

photooxidation $t_{1/2} = 14.5\text{--}145$ h in air, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 440$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992);

phototransformation decay $k = 0.15 \text{ min}^{-1}$ on 0.20 g/L of TiO_2 solution (Minero et al. 1993).

Hydrolysis:

Biodegradation: 95% degradation in 3–6 d in mixture bacteria cultures (Tabak et al. 1964);

decomposition by a soil microflora in 16 d (Alexander & Lustigman 1966; quoted, Verschueren 1983);

average rate of biodegradation $17.5 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

time necessary for complete degradation of 16 mg/L in 3–5 d by wastewater and 7–14 d by soil (Haller 1978);

aqueous aerobic $t_{1/2} = 18.2\text{--}168$ h, based on pond die-away test data (Paris et al. 1983; Bourquin 1984; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 163\text{--}235$ h, based on anaerobic die-away data in two different flooded soils (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991);

was not biodegraded with activated sludge at a concn. of 94 mg/L but completely degraded with a decreased concn. of 19 mg/L in 28 d expt. (Kool 1984).

Biotransformation: estimated bacterial transformation rate constant of $1.00 \times 10^{-7} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982);

rate constant of $(3.80 \pm 1.40) \times 10^{-11} \text{ L}\cdot\text{organism}^{-1}\cdot\text{h}^{-1}$ (Paris et al. 1983; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 14.5\text{--}145$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1–5 to > 5 d (Kelly et al. 1994).

Surface water: photodegradation $t_{1/2} = 5.7$ d at pH 5, $t_{1/2} = 6.7$ d at pH 7 and $t_{1/2} = 13.7$ d at pH 9 in water (Hustert et al. 1981);

$t_{1/2} = 1\text{--}8$ d in freshwater, $t_{1/2} = 1\text{--}3$ yr in marine systems but decreased to 13–20 d with the presence of sediment, the mean $t_{1/2} = 7.7$ d estimated by a nonsteady-state equilibrium model, and photolysis $t_{1/2} = 2\text{--}14$ d in clear surface waters (Howard 1989);

$t_{1/2} = 18.2\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991);

$t_{1/2} = 440$ min for photolysis in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Groundwater: $t_{1/2}$ = 36.4–235 h, based on pond die-away test data and anaerobic die-away data in two different flooded soils (Paris et al. 1983; Sudhakar-Barik & Sethunnathan 1978; quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2}$ ~ 1 d in agricultural topsoil and $t_{1/2}$ = 10 d in flooded soil, $t_{1/2}$ > 40 d in subsoil under aerobic conditions and longer still under anaerobic conditions (Howard 1989);

$t_{1/2}$ = 17–29 h, based on aerobic soil die-away test data (Loecke 1985; selected, Howard et al. 1998).

$t_{1/2}$ = 75 d in a coarse sandy soil, $t_{1/2}$ = 145 d in sandy loam (Kjeldsen et al. 1990)

Biota: depuration $t_{1/2}(\text{obs.})$ = 72 h, $t_{1/2}(\text{calc.})$ = 37 h for mean exposure level of $0.0041 \mu\text{g}\cdot\text{mL}^{-1}$ and $t_{1/2}(\text{obs.})$ = 228 h, $t_{1/2}(\text{calc.})$ = 206 h for mean exposure level of $0.041 \mu\text{g}\cdot\text{mL}^{-1}$ (Call et al. 1980).

TABLE 14.1.3.3.1

Reported aqueous solubilities of 4-nitrophenol at various temperatures

Sidgwick et al. 1915		Achard et al. 1996		Beneš & Dohnal 1999		Jaoui et al. 2002	
shake flask-synthetic method		shake flask-conductimetry		shake flask-UV spec.		shake flask-optical method	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
34.8	29100	15.3	10162	10	8050	12.75	8694
37.2	31100	25.0	15599	20	12000	18.15	11477
40.4	33400	30.3	29600	30	17800	23.65	15052
47.7	39300	34.9	28845	38	23900	34.55	25082
51.2	43000					41.05	33428
59.1	53300			mp/K	386.95	14.65	9599
67.8	69900			$\Delta H_{\text{fus}}/(\text{kJ mol}^{-1}) = 18.25$		19.65	12367
72.6	82800			Enthalpies of solution*:		25.35	16345
79.3	106100	OECD 1981		$\Delta H_{\text{sol}}(\text{solid}) = 28.9 \text{ kJ mol}^{-1}$		33.55	23969
84.4	137000	shake flask (6 laboratories)		$\Delta H_{\text{sol}}(\text{liq.}) = 16.9 \text{ kJ mol}^{-1}$		39.25	30896
87.9	175300	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$			11.15	7999
90.2	215800	15	9950 [†]			15.85	10211
91.3	261600	25	14800 [‡]			23.15	14690
92.3	304100					34.55	25082
92.8	331900	[†] mean, 8880–10900 $\text{g}\cdot\text{m}^{-3}$				40.65	32844
...	...	[‡] mean, 13800–15900 $\text{g}\cdot\text{m}^{-3}$					
critical solution temp 92.8°C							
triple point 39.6°C							

*Enthalpies of solution at infinite dilution for solid at environmental temperatures and for hypothetical liquid.

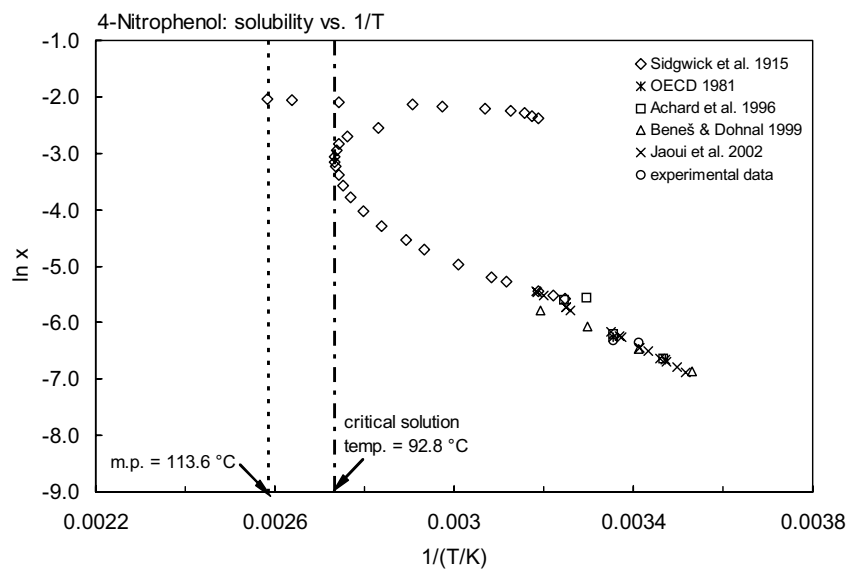
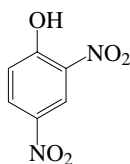


FIGURE 14.1.3.3.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 4-nitrophenol.

14.1.3.4 2,4-Dinitrophenol



Common Name: 2,4-Dinitrophenol

Synonym: 2,4-hydroxynitrobenzene, Aldifen, 2,4-DNP

Chemical Name: 2,4-dinitrophenol

CAS Registry No: 57-28-5

Molecular Formula: $C_6H_4N_2O_5$, $C_6H_3(NO_2)_2OH$

Molecular Weight: 184.106

Melting Point ($^{\circ}C$):

114.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

sublimation (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.684 ($24^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

160.4 (calculated-Le Bas method at normal boiling point)

Acid Dissociation Constant, pK_a :

4.09 (Pearce & Simkins 1968)

3.94 (Schwarzenbach et al. 1988; Haderlein & Schwarzenbach 1993)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$, F : 0.132 (mp at $114.8^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

6000 (Morrison & Boyd 1959, Howard 1989)

5600 ($18^{\circ}C$, Verschueren 1977)

335* ($20 \pm 0.5^{\circ}C$, shake flask-UV at pH 1.5, Schwarzenbach et al. 1988)

2787 ($20 \pm 0.5^{\circ}C$, supercooled liquid S_L , Schwarzenbach et al. 1988)

5000 (selected, Brecken-Folse et al. 1994; Howe et al. 1994)

560 (solid-phase microextraction SPME-GC, Buchholz & Pawliszyn 1994)

691* (shake flask-conductimetry, measured range 15.1 – $35^{\circ}C$, Achard et al. 1996)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

5.52×10^{-3} (Knudsen effusion method, Hoyer & Peperle 1958)

$\log(P/mmHg) = 13.95 - 5466/(T/K)$, temp range 20 – $60^{\circ}C$ (Knudsen effusion method, Hoyer & Peperle 1958)

1.987×10^{-3} ($18^{\circ}C$, Mabey et al. 1982)

5.520×10^{-3} (Interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_S/kPa) = 13.075 - 5466/(T/K)$, temp range 291 – $333\ K$ (solid, Antoine eq., Stephenson & Malanowski 1987)

0.111 ($20^{\circ}C$: supercooled liquid P_L , GC-RT correlation, Schwarzenbach et al. 1988)

0.0207 ($20^{\circ}C$: solid P_S , converted from P_L with ΔS_{fus} and mp, Schwarzenbach et al. 1988)

$\log(P_L/atm) = 7.392 - 3680/(T/K)$ (Antoine eq., GC-RT correlation, Schwarzenbach et al. 1988)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.54×10^{-5} ($18^{\circ}C$, calculated-P/C, Mabey et al. 1982)

0.00335 ($20^{\circ}C$, calculated-P/C, Schwarzenbach et al. 1988)

8.880×10^{-5} (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, log K_{OW} :

1.53	(Leo et al. 1971)
1.50	(shake flask-UV, Stockdale & Selwyn 1971)
1.54	(shake flask-GC, Kurihara et al. 1973)
1.56	(shake flask-UV, Korenman et al. 1977)
1.52	(QSAR, Scherrer & Howard 1979)
1.55	(shake flask-UV, Terada et al. 1981)
1.79 \pm 0.06	(HPLC-RV correlation-ALPM, Garst 1984)
1.51	(shake flask, Log P Database, Hansch & Leo 1987)
1.67	(21 \pm 1.5°C, shake flask-UV, both phases, Schwarzenbach et al. 1988)
1.54	(recommended, Sangster 1993)
1.53	(22°C, shake flask, Brecken-Folse et al. 1994)
-0.23	(shake flask, pH 7.5, Howe et al. 1994)
1.67	(recommended, Hansch et al. 1995)

Bioconcentration Factor, log BCF:

1.19	(microorganism-water, calculated- K_{OW} , Mabey et al. 1982)
< 1.0	(calculated, Howard 1989)

Sorption Partition Coefficient, log K_{OC} :

1.22	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
1.56, 2.14	(calculated-S, K_{OW} , Howard 1989)
-0.09	(calculated- K_{OW} , Kollig 1993)
3.09	(activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: aqueous oxidation rate constants $k = 3 \times 10^4 \text{ M}^{-1}\cdot\text{h}^{-1}$ for singlet oxygen, and $k = 5 \times 10^5 \text{ M}^{-1}\cdot\text{h}^{-1}$ for peroxy radical (Mabey et al. 1982);

photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 111\text{--}1114 \text{ h}$ in air, based on the estimated reaction rate constant $k = 1.7 \times 10^{-11} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ with an ambient hydroxyl radical concentration of $8 \times 10^5 \text{ molecules}\cdot\text{cm}^{-3}$ for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 200 \text{ min}$ in the presence of hydrogen peroxide irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992).

Hydrolysis:

Biodegradation: 95% degradation in 7–10 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $6.0 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

first-order rate constant $k = 0.2 \text{ d}^{-1}$ corresponding to a $t_{1/2} = 3.6 \text{ d}$ in adapted activated sludge under aerobic conditions (Mills et al. 1982);

aqueous aerobic $t_{1/2} = 1622\text{--}6312 \text{ h}$, based on data from aerobic soil column studies (Kincannon & Lin 1985; selected, Howard et al. 1991) and aerobic soil die-away test data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)

aqueous anaerobic $t_{1/2} = 68\text{--}170 \text{ h}$, based on anaerobic flooded soil die-away tests (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 68 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2.8 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: bacterial transformation rate constant $k = 3 \times 10^{-9} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: calculated vapor-phase $t_{1/2} = 14 \text{ h}$ for reaction with photochemically generated OH radical (Howard 1989)

photooxidation $t_{1/2} = 111\text{--}1114$ h, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be > 5 d (Kelly et al. 1994).

Surface water: calculated $t_{1/2} = 58$ d for reaction with alkylperoxy radical in water (Howard 1989);

$t_{1/2} = 77\text{--}3840$ h, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 200$ min in the presence of hydrogen peroxide, irradiated with a mercury-xenon lamp (Lipczynska-Kochany 1992)

$t_{1/2}(\text{aerobic}) = 69$ d, $t_{1/2}(\text{anaerobic}) = 2.8$ d in natural waters (Capel & Larson 1995)

Groundwater: $t_{1/2} = 68\text{--}14624$ h, based on estimated aqueous aerobic biodegradation half-life and estimated aqueous anaerobic biodegradation half-life (quoted, Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 1622\text{--}6312$ h, based on data from aerobic soil column studies (Kincannon & Lin 1985) and aerobic soil die-away test data (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991);

a Class C compounds with a $t_{1/2} > 50$ d in soil (Ryan et al. 1988).

$t_{1/2} = 145$ d in sandy loam (Kjeldsen et al. 1990)

Biota:

TABLE 14.1.3.4.1

Reported aqueous solubilities of 2,4-dinitrophenol at various temperatures

Schwarzenbach et al. 1988				Achard et al. 1996	
shake flask-UV spec.				shake flask-conductimetry	
$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
	solid		supercooled liquid		
5	171.8	0	2019	15.1	415
10	206.6	10	2213	25.0	691
20	335.0	20	2852	35.0	975
30	473.2	30	3199		

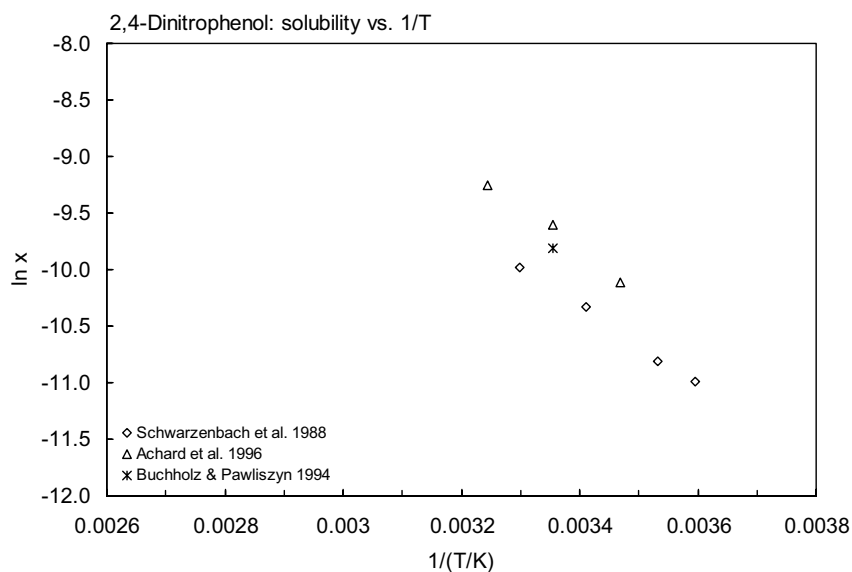
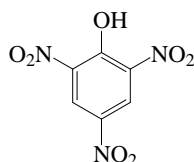


FIGURE 14.1.3.4.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for 2,4-dinitrophenol.

14.1.3.5 2,4,6-Trinitrophenol (Picric acid)



Common Name: 2,4,6-Trinitrophenol

Synonym: Picric acid

Chemical Name: 2,4,6-trinitrophenol

CAS Registry No: 88-89-1

Molecular Formula: $C_6H_3N_3O_7$, $C_6H_2(NO_2)_3OH$

Molecular Weight: 229.104

Melting Point ($^{\circ}C$):

122.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

> 300 (explodes, Weast 1982–83; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.763 (Weast 1982–83; Dean 1985)

Acid Dissociation Constant, pK_a :

0.78 (Schwarzenbach et al. 1988)

Molar Volume (cm^3/mol):

188.9 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

19.50 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

49.37 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.111 (mp at $122.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

14000 (Morrison & Boyd 1959)

13750 (selected, Tsonopoulos & Prausnitz 1971)

14000 ($20^{\circ}C$, Verschueren 1983)

13000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.68×10^{-5} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.319 - 5560/(T/K)$, temp range 468–598 K (liquid, Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

7.66×10^{-7} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.44 (shake flask-GC, Korenman et al. 1977)

1.34 (Scherrer & Howard 1979)

1.46 (HPLC-RV correlation, Garst 1984)

–0.97, 0.87 (shake flask, Log P database: pH 2.7, pH 1, Hansch & Leo 1987)

2.03 (shake flask, Log P Database, Hansch Leo 1987)

1.33 (recommended, Sangster 1993)

1.82 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 677\text{--}4320$ h, based on estimated reaction rates with OH and NO₃ radicals in air (Howard et al. 1991).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: 95% degradation in 3–6 d in mixed bacteria cultures (Tabak et al. 1964);

aqueous aerobic $t_{1/2} = 672\text{--}8640$ h, based on aerobic biodegradation screening test (Howard et al. 1991);
aqueous anaerobic $t_{1/2} = 48\text{--}300$ h, based on aqueous anaerobic natural water die-away test data (Howard et al. 1991)

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{1/2} = 672\text{--}4320$ h, based on estimated photooxidation half-lives in air (Howard et al. 1991).

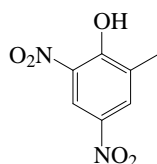
Surface water: $t_{1/2} = 672\text{--}4320$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}8640$ h, based on estimated both aqueous aerobic and aqueous anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 672\text{--}4320$ h, based on estimated photooxidation aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biota:

14.1.3.6 4,6-Dinitro-*o*-cresol

Common Name: 4,6-Dinitro-*o*-cresol

Synonym: 2,4-dinitro-6-methylphenol, DNOC, 2-methyl-4,6-dinitrophenol, 6-methyl-2,4-dinitrophenol

Chemical Name: 4,6-dinitro-*o*-cresol, 2,4-dinitro-6-methylphenol

CAS Registry No: 534-52-1

Molecular Formula: $C_7H_6N_2O_5$, $CH_3C_6H_2(NO_2)_2OH$

Molecular Weight: 198.133

Melting Point ($^{\circ}C$):

86.5 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

312 (Howard 1991)

Density (g/cm^3 at $20^{\circ}C$):

Acid Dissociation Constant, pK_a :

4.35 (Pearce & Simkins 1968; Callahan et al. 1979; Westall et al. 1985)

4.31 (Schwarzenbach et al. 1988; Howard 1991)

4.46 (Jafvert 1990; quoted, Bintein & Devillers 1994)

Molar Volume (cm^3/mol):

182.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$, $F: 0.249$ (mp at $86.5^{\circ}C$))

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

258, 250 (Günther et al. 1968)

290 (calculated- K_{ow} , Mabey et al. 1982)

198 ($20^{\circ}C$, neutral species at pH 1.5 of buffer solution HCl/NaH_2PO_4 , shake flask-UV, Schwarzenbach et al. 1988)

150 ($20^{\circ}C$, quoted, Howard 1991)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.048 ($35^{\circ}C$, Knudsen effusion method, Hamaker & Kerlinger 1969)

6.670 ($20^{\circ}C$, estimated, Mabey et al. 1982)

0.0142 (interpolated-Antoine eq., solid, Stephenson & Malanowski 1987)

$\log(P_s/kPa) = 13.265 - 5400/(T/K)$; temp range 290–324 K (Antoine eq., solid, Stephenson & Malanowski 1987)

0.240 ($20^{\circ}C$, GC-RT correlation, supercooled liquid value P_L , Schwarzenbach et al. 1988)

0.0432 ($20^{\circ}C$, solid P_s , Schwarzenbach et al. 1988)

0.0111 ($20^{\circ}C$, quoted, Howard 1991)

Henry's Law Constant ($Pa \cdot m^3/mol$):

4.050 (calculated- P/C , Mabey et al. 1982)

43.22 ($20^{\circ}C$, calculated- P/C , Schwarzenbach et al. 1988)

Octanol/Water Partition Coefficient, $\log K_{ow}$ at $25^{\circ}C$ or as indicated:

2.70 (calculated-fragment const., Mabey et al. 1982)

2.12 ($21.5^{\circ}C$, neutral species, shake flask-UV, Schwarzenbach et al. 1988)

−0.81 ($21.5^{\circ}C$, ionic species at pH 12, Schwarzenbach et al. 1988)

2.12 (Howard 1991)

- 2.12 (Sangster 1993)
2.56, 1.98 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

- 2.10 (microorganism-water, calculated- K_{OW} , Mabey et al. 1982)
1.38, 1.57 (calculated-S, K_{OW} regression equations., Howard 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.38 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 3.57 ± 0.130 (natural sediment, Jafvert 1990)
2.44, 2.0–2.53 (calculated-S, K_{OW} regression eq., Howard 1991)
2.41, 2.78 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
3.28 (activated carbon, Blum et al. 1994)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization: nonvolatile from water, based on low Henry's law constant value (Howard 1991).

Photolysis:

Oxidation: aqueous oxidation rate constant $k = 3 \times 10^4 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 5 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical at 25°C (Mabey et al. 1982);
photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
photooxidation $t_{1/2} = 310\text{--}3098 \text{ h}$ in air, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: aqueous aerobic $t_{1/2} = 168\text{--}504 \text{ h}$, based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 68\text{--}170 \text{ h}$, based on flooded soil die-away tests for 2,4-dinitrophenol (Sudhakar-Barik & Sethunnathan 1978; selected, Howard et al. 1991)
 $t_{1/2}(\text{aerobic}) = 7 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

Biotransformation: estimated bacterial transformation rate constant $k = 3 \times 10^9 \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ in water (Mabey et al. 1982).

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 310\text{--}3098 \text{ h}$ in air, based on estimated rate constant for the vapor phase reaction with OH radical in air (Atkinson 1987; selected, Howard et al. 1991);
 $t_{1/2} = 77 \text{ d}$ for the vapor-phase reaction with OH radical (concn. of $5 \times 10^5 \text{ molecule}\cdot\text{cm}^{-3}$) (Howard 1991);
atmospheric transformation lifetime was estimated to be $> 5 \text{ d}$ (Kelly et al. 1994).

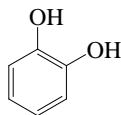
Surface water: photooxidation $t_{1/2}$ of $77\text{--}3840 \text{ h}$ in water, based on reported reaction rate constants for RO_2 radical with the phenol class (Mill & Mabey 1985; selected, Howard et al. 1991);
 $t_{1/2} \sim 58 \text{ d}$, estimated for photooxidation via peroxy radicals and $t_{1/2} = 2600 \text{ yr}$ for reaction with singlet oxygen in water (Howard 1991)
 $t_{1/2}(\text{aerobic}) = 7 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2.8 \text{ d}$ in natural waters (Capel & Larson 1995)

Ground water: $t_{1/2} = 68\text{--}1008 \text{ h}$, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}504 \text{ h}$, based on data from a soil die-away study (Kincannon & Lin 1985; selected, Howard et al. 1991).

Biota:

14.1.4 DIHYDROXYBENZENES, METHOXYPHENOLS AND CHLOROGUAIACOLS**14.1.4.1 Catechol (1,2-Dihydroxybenzene)**

Common Name: Catechol

Synonym: 1,2-dihydroxybenzene, 1,2-benzenediol, pyrocatechol

Chemical Name: 1,2-dihydroxybenzene

CAS Registry No: 120-80-9

Molecular Formula: $C_6H_4(OH)_2$

Molecular Weight: 110.111

Melting Point ($^{\circ}C$):

104.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

245 (Weast 1982–83; Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

1.1493 (22 $^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.40 (Fieser & Fieser 1958)

9.50 (McLeese et al. 1979)

Molar Volume (cm^3/mol):

110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

22.76 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

60.25 (Tsonopoulos & Prausnitz 1971)

60.21 (Yalkowsky & Valvani 1980)

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.166 (mp at 104.6 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$ or as indicated):

71166 (30 $^{\circ}C$, synthetic method, Walker et al. 1931)

45000 (Fieser & Fieser 1958; Morrison & Boyd 1959)

636190 (quoted, Tsonopoulos & Prausnitz 1971)

35630 (calculated- K_{OW} , Yalkowsky & Morozowich 1980)

42724, 38610 (calculated- ΔS_{fus} and mp, estimated, Yalkowsky & Valvani 1980)

43000 (Dean 1985)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

666.6* (104 $^{\circ}C$, summary of literature data, temp range 104–245.5 $^{\circ}C$, Stull 1947)

1333* (118.5 $^{\circ}C$, ebulliometry, measured range 118.5–245.5 $^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 13779.7/(T/K)] + 8.694319$; temp range 104–245.5 $^{\circ}C$ (Antoine eq., Weast 1972–73)

1.34 (extrapolated-Antoine eq., Boublik et al. 1973)

$\log(P/mmHg) = 7.57299 - 2024.422/(186.533 + t/^{\circ}C)$; temp range 118.5–245.5 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1973)

$\log(P/mmHg) = [1 - 517.477/(T/K)] \times 10^{0.902426 - 6.04783 \times 10^{-4} \cdot (T/K) + 6.58278 \times 10^{-7} \cdot (T/K)^2}$; temp range: 377.15–518.65 K, (Cox eq., Chao et al. 1983)

5.44 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.9896 - 3144.241/(281.825 + t/^{\circ}C)$; temp range 118.5–245.5 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

1.03(extrapolated-Antoine eq., Dean 1985)

$\log (P/\text{mmHg}) = 7.577 - 2054/(187.0 + t/^{\circ}\text{C})$; temp range 118–246°C (Antoine eq., Dean 1985, 1992)

1.06(P_L , extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.61028 - 1954.6/(-94.25 + T/\text{K})$; temp range 395–519 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.022 (calculated-P/C)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.86 (shake flask-UV, Fujita et al. 1964)
 0.95 (Leo et al. 1971)
 0.85 (shake flask-UV, pH 5.6, Umeyama et al. 1971)
 0.84 (shake flask, Korenman 1972)
 0.86 (shake flask at pH 7, Unger et al. 1978)
 0.88, 1.01, 0.85, 0.84 (literature values, Hansch & Leo 1979)
 0.95 (GC-RT correlation, Veith et al. 1979)
 1.10 (HPLC-RT correlation, Butte et al. 1981)
 0.53 (HPLC- k' correlation, Haky & Young 1984)
 1.10 (HPLC-RT correlation, Webster et al. 1985)
 0.88 (recommended, LOGKOW databank, Sangster 1993)
 0.88 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

2.03 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
 1.42; 1.74, 2.25, 2.01, 1.98, 1.82 (soil: calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $t_{1/2} < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

photooxidation $t_{1/2} = 2.6\text{--}26 \text{ h}$ in air, based on vapor-phase reaction rate constant with OH radical in atmosphere (Howard et al. 1991);

aqueous photooxidation $t_{1/2} = 77\text{--}3840 \text{ h}$, based on reaction rate constant for RO_2^- radical in aqueous solution (Mill & Mabey 1985; selected, Howard et al. 1991).

Hydrolysis:

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $k = 55.5 \text{ mg COD g}^{-1} \cdot \text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

2 mM catechol rapidly degraded by strain Cat $_{1/2}$ in batch culture in 9 d (Schnell et al. 1989);

aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on aerobic biological screening test data (Heukelekian & Rand 1955; Okey & Bogan 1965; Pitter 1976; Urushigawa et al. 1983; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated photooxidation half-lives in air (Atkinson 1987; selected, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168 \text{ h}$, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-lives (Howard et al. 1991).

Biota:

TABLE 14.1.4.1.1

Reported vapor pressures of catechol (1,2-dihydroxybenzene) at various temperatures

Stull 1947		Vonterres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
104.0	666.6	118.5	1333
118.3	1333	139.3	3333
134.0	2666	157.0	6666
150.6	5333	168.0	9999
161.7	7999	176.2	13332
176.0	13332	188.2	19998
197.7	26664	198.0	26664
221.5	53329	204.0	33330
245.5	101325	210.9	39997
		213.3	43330
mp/°C	105	215.8	46663
		220.0	53329
		224.6	59995
		228.2	66661
		231.4	73327
		235.0	79993
		237.8	86659
		241.0	93325
		245.5	101327
		bp/°C	243.823

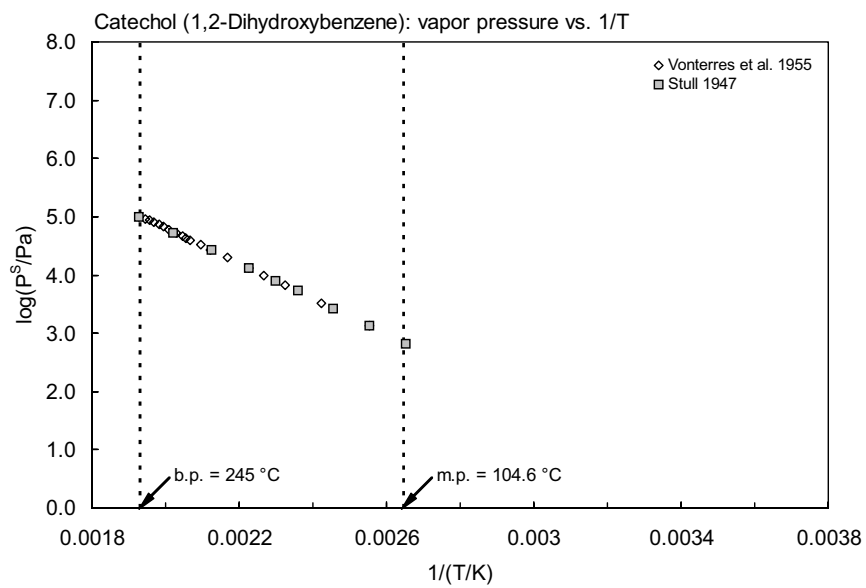
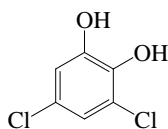


FIGURE 14.1.4.1.1 Logarithm of vapor pressure versus reciprocal temperature for catechol.

14.1.4.2 3,5-Dichlorocatechol



Common Name: 3,5-Dichlorocatechol

Synonym:

Chemical Name: 3,5-dichlorocatechol

CAS Registry No: 13673-92-2

Molecular Formula: $C_6H_4Cl_2O_2$, $C_6H_2Cl_2(OH)_2$

Molecular Weight: 179.001

Melting Point ($^{\circ}C$):

83–84 (Varhaníčková 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constants, pK_a :

7.78 (Varhaníčková 1995)

Molar Volume (cm^3/mol):

152.6 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7910 (at pH 4.70. shake flask-HPLC/UV, Varhaníčková 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

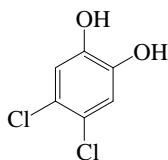
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.3 4,5-Dichlorocatechol



Common Name: 4,5-Dichlorocatechol

Synonym:

Chemical Name: 4,5-dichlorocatechol

CAS Registry No: 3428-24-8

Molecular Formula: $C_6H_4Cl_2O_2$, $C_6H_2Cl_2(OH)_2$

Molecular Weight: 179.001

Melting Point ($^{\circ}C$):

116–117 (Varhanířková 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

8.17 (Varhanířková 1995)

Molar Volume (cm^3/mol):

152.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

12000 (at pH 3.20, shake flask-HPLC/UV, Varhanířková 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations

0.408 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3680/(T/K) - 11.95$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.00078 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.51–2.93 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

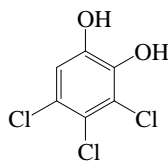
1.18–1.51 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.4 3,4,5-Trichlorocatechol



Common Name: 3,4,5-Trichlorocatechol

Synonym: 3,4,5-trichloro-1,2-benzenediol

Chemical Name: 3,4,5-trichlorocatechol

CAS Registry No: 56961-20-7

Molecular Formula: $C_6H_3Cl_3O_2$, $C_6HCl_2(OH)_2$

Molecular Weight: 213.446

Melting Point ($^{\circ}C$):

130 (Varhaníčková 1995)

134 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a : 6.95 (Varhaníčková 1995)

Molar Volume (cm^3/mol):

173.5 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

79.3 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 0.085 (mp at $134^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

511 (at pH 4.05, shake flask-HPLC/UV, Varhaníčková 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.106 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4135/(T/K) - 12.89$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.79, 3.71 (shake flask-GC, HPLC-RT correlation, Xie et al. 1984)

3.89, 3.17 (calculated- π constant, fragment constant, Xie et al. 1984)

3.71 (HPLC-RT correlation, Xie et al. 1984; quoted, Sangster 1993)

3.75 (quoted, NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.16 (estimated- K_{OW} , NCASI 1992)

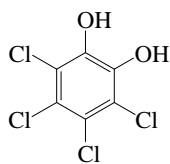
Sorption Partition Coefficient, $\log K_{OC}$:

4.35 (sediment, $K_p = 22 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.5 Tetrachlorocatechol



Common Name: Tetrachlorocatechol

Synonym: 3,4,5,6-tetrachloro-1,2-benzenediol

Chemical Name: tetrachlorocatechol

CAS Registry No: 1198-55-6

Molecular Formula: $C_6H_2Cl_4O_2$, $C_6Cl_4(OH)_2$

Molecular Weight: 247.891

Melting Point ($^{\circ}C$):

194 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

5.83 (Varhaníčková 1995)

Molar Volume (cm^3/mol):

194.4 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.9 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.022 (mp at $194^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

70.5 (at pH 5.13, shake flask-HPLC/UV, Varhaníčková 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.068 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -4070/(T/K) - 12.48$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

0.035 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.29 (shake flask-GC, Fujita et al. 1964)

4.27 (HPLC-RT correlation, Saarikoski & Viluksela 1982)

4.19, 4.27 (shake flask-GC, HPLC-RT correlation, Xie et al. 1984)

4.29 (recommended, Sangster 1993)

4.29 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.54 (estimated- K_{ow} , NCASI 1992)

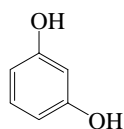
Sorption Partition Coefficient, $\log K_{OC}$:

4.56 (sediment, $K_p = 36.1 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.6 Resorcinol (1,3-Dihydroxybenzene)



Common Name: Resorcinol

Synonym: 1,3-benzenediol, *m*-dihydroxybenzene, *m*-hydroxyphenol, resorcin

Chemical Name: 1,3-dihydroxybenzene

CAS Registry No: 108-46-3

Molecular Formula: $C_6H_6O_2$, $C_6H_4(OH)_2$

Molecular Weight: 110.111

Melting Point ($^{\circ}C$):

109.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

276.5 (Lide 2003)

Density (g/cm^3):

1.2717 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.40 (Fieser & Fieser 1958; McLeese et al. 1979)

Molar Volume (cm^3/mol):

110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

21.30 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

55.65 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.149 (mp at $109.4^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

2188900 ($33.6^{\circ}C$, synthetic method, Walker et al. 1931)

1230000 (Fieser & Fieser 1958; Morrison & Boyd 1959)

1309000 (Tsonopoulos & Prausnitz 1971)

840000, 2290000 (0, $30^{\circ}C$, Verschueren 1983)

110000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.3300* (extrapolated-regression of tabulated data, temp range 108.4 – $276.5^{\circ}C$, Stull 1947)

1333* ($151.5^{\circ}C$, ebulliometry, measured range 151.5 – $276.5^{\circ}C$, Vonterres et al. 1955)

0.0118 (Knudsen method, calculated-Antoine eq., Hoyer & Peperle 1958)

$\log (P/mmHg) = [-0.2185 \times 16400.8/(T/K)] + 9.413304$; temp range 108.4 – $276.5^{\circ}C$ (Antoine eq., Weast 1972–73)

0.0280* (gas saturation, extrapolated-Antoine eq., measured range 55 – $106^{\circ}C$, Bender et al. 1983)

$\log (P/mmHg) = [1 - 549.041/(T/K)] \times 10^{\{0.958295 - 5.78954 \times 10^{-4} \cdot (T/K) + 6.46841 \times 10^{-7} \cdot (T/K)^2\}}$; temp range 381.55 – $549.65\ K$ (Cox eq., Chao et al. 1983)

0.0515 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 7.16673 - 2359.273/(180.962 + t/^{\circ}C)$; temp range 151.5 – $216.5^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.0300 (extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 7.889 - 2231/(169.0 + t/^{\circ}C)$, temp range 151 – $276^{\circ}C$ (Antoine eq., Dean 1985, 1992)

0.0118 (P_s , interpolated-Antoine eq.-I, temp range 10 – $50^{\circ}C$, Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 11.425 - 4876/(T/K)$; temp range 283 – $323\ K$ (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.52635 - 1918.1/(-128.65 + T/\text{K})$; temp range 419–550 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.1041 - 1745.2/(-133.81 + T/\text{K})$; temp range 392–463 K (Antoine eq.-III, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$):

4.0×10^{-8} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.80 (shake flask-UV, Fujita et al. 1964; Leo et al. 1969)

0.78 (20°C, shake flask-UV, Korenman 1972)

0.80, 0.77, 0.78 (Hansch & Leo 1979)

0.77 (shake flask-UV, Beezer et al. 1980)

0.88 (shake flask-HPLC both phases, Nahum & Horvath 1980)

0.36 (HPLC-RT correlation, Butte et al. 1981)

0.77 (shake flask, Log P Database, Hansch & Leo 1987)

0.82 (HPLC-RT correlation, Minnick et al. 1988)

0.79 (shake flask-UV, pH 2-8, Wang et al. 1989)

0.80 (COMPUTOX, Kaiser 1993)

0.80 (recommended, Sangster 1993)

0.72 ± 0.15 (solvent generated liquid-liquid chromatography SGLLC-correlation, Cichna et al. 1995)

0.80 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: measured pseudo-first-order reaction rate constant $k = 0.014 \text{ min}^{-1}$ for direct photolysis in aqueous solutions with $t_{1/2} = 50.7 \text{ min}$. (Peijnenburg et al. 1992).

Photooxidation: rate constant $k > 3 \times 10^5 \text{ M}^{-1}\cdot\text{s}^{-1}$ for the reaction with ozone in water using 1 mM *t*-BuOH as scavenger at pH 2.0 and 20–23°C in water (Hoigné & Bader 1983a,b).

Hydrolysis:

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $k = 57.5 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

2 mM resorcinol solution degraded by strain Re10 within 4 d (Schnell et al. 1989).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air:

Surface water: $t_{1/2} = (50.7 \pm 1.0) \text{ min}$ for directly photolysis in aqueous solutions (Peijnenburg et al. 1992).

Ground water:

Sediment:

Soil:

Biota:

TABLE 14.1.4.6.1

Reported vapor pressures of resorcinol (1,3-dihydroxybenzene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)			
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Vonterres et al. 1955		Bender et al. 1983	
summary of literature data		ebulliometry		gas saturation-IR	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
					solid
108.4	133.3	151.5	1333	55.35	0.86
138.0	666.6	175.0	3333	66.35	2.73
152.1	1333	190.3	6666	76.45	6.94
168.0	2666	201.7	9999	85.45	14.4
185.3	5333	210.0	13332	92.65	29.2
195.8	7999	221.7	19998	100.05	50.8
209.8	13332	230.1	26664	105.95	81.3
230.8	26664	237.0	33330		
253.4	53329	240.2	39997		
276.5	101325	246.0	43330	eq. 1a	P ^s /Pa
		248.0	46663	A	33.807
mp/°C	110.7	252.0	53329	B	11147
		257.0	59995		
		261.0	66661		
		264.0	73327		
		267.0	79993		
		270.0	86659		
		273.0	93325		
		276.5	101325		
		bp/°C	276.205		

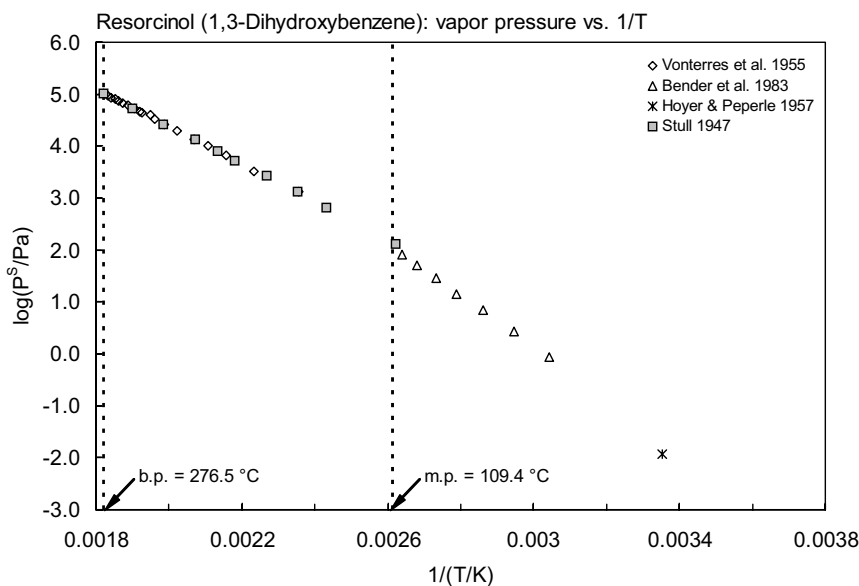
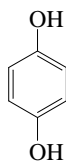


FIGURE 14.1.4.6.1 Logarithm of vapor pressure versus reciprocal temperature for resorcinol.

14.1.4.7 Hydroquinone (1,4-Dihydroxybenzene)



Common Name: Hydroquinone

Synonym: 1,4-benzenediol, *p*-dihydroxybenzene, *p*-hydroxyphenol, quinol, hydroquinol

Chemical Name: 1,4-dihydroxybenzene

CAS Registry No: 123-31-9

Molecular Formula: $C_6H_4(OH)_2$

Molecular Weight: 110.111

Melting Point ($^{\circ}C$):

172.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Weast 1982–83; Lide 2003)

Density (g/cm^3):

1.328 (15 $^{\circ}C$, Weast 1982–83)

Acid Dissociation Constant, pK_a :

9.90 (McLeese et al. 1979)

Molar Volume (cm^3/mol):

110.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

27.11 (Tsonopoulos & Prausnitz 1971)

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

60.67 (Tsonopoulos & Prausnitz 1971)

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F : 0.036 (mp at 172.4 $^{\circ}C$)

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

73700 (synthetic method, Walker et al. 1931)
 80140 (shake flask-interferometry, Korman & La Mer 1936)
 80000 (Fieser & Fieser 1958; Morrison & Boyd 1959)
 80750 (selected, Tsonopoulos & Prausnitz 1971)
 70000 (20–25 $^{\circ}C$, Geyer et al. 1981)
 70000 (Rott et al. 1982; Verschuereen 1983; Dean 1985)
 86450 (Windholz 1983)

Vapor Pressure (Pa at 25 $^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* (132.4 $^{\circ}C$, summary of literature data, temp range 132.4–286.2 $^{\circ}C$, Stull 1947)

$\log (P/mmHg) = [-0.2185 \times 18734.0/(T/K)] + 10.309301$; temp range 132.4–286.2 $^{\circ}C$ (Antoine eq., Weast 1972–73)

0.00276* (gas saturation, extrapolated - Antoine eq., measured range 68–126 $^{\circ}C$, Bender et al. 1983)

$\log (P/mmHg) = [1 - 558.031/(T/K)] \times 10^{0.941185 - 5.32724 \times 10^{-4} \cdot (T/K) + 5.41185 \times 10^{-7} \cdot (T/K)^2}$; temp range: 432.25–559.15 K, (Cox eq., Chao et al. 1983)

0.03940 (extrapolated - liquid, Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 7.41617 - 2397.626/(194.743 + t/^{\circ}C)$; temp range 159.1–286 $^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

0.00255 (P_s , interpolated, Antoine eq., Stephenson & Malanowski 1987)

$\log (P_s/kPa) = 12.585 - 5420/(T/K)$; temp range 298–346 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 7.00575 - 2321.92/(-95.235 + T/K)$; temp range 448–559 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

3.89×10^{-6} (quoted, Meylan & Howard 1991)

5.91×10^{-6} (estimated-bond contribution, Meylan & Howard 1991)

4.00×10^{-6} (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.59 (Leo et al. 1971)

0.495 (shake flask-UV at pH 5.62, Umeyama et al. 1971)

0.59 (shake flask-GC, Kurihara et al. 1973)

0.61 (20°C , shake flask, Korenman 1974)

0.55, 0.59 (shake flask, OECD 1981 Guidelines, Geyer et al. 1984)

0.61 (HPLC-RT correlation, Nahum & Horvath 1980)

0.54 (shake flask-HPLC, Nahum & Horvath 1980)

0.99 (HPLC-RT correlation, Fujisawa & Masuhara 1981)

0.50 (shake flask, Log P Database, Hansch & Leo 1987)

0.50 (centrifugal partition chromatography CPC, Berthod et al. 1988)

0.59 (shake flask, Wang et al. 1989)

0.59 (recommended, Sangster 1993)

0.59 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

1.81 (green algae, *Chlorella*, exposure to $50 \mu\text{g/L}$ for 24 h, Geyer et al. 1981)

0.95 (calculated-S, Geyer et al. 1981)

1.60, 2.72 (golden orfe, activated sludge, Freitag et al. 1982)

1.60, 1.60 (algae, fish, Freitag et al. 1984)

1.54 (algae, wet weight basis after 1 d, Geyer et al. 1984)

0.602 (calculated- K_{OW} , Geyer et al. 1984)

2.93 (activated sludge, Freitag et al. 1987)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: $k = 1 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with RO_2 radical at 30°C in aquatic systems with $t_{1/2} = 12 \text{ min}$ (Howard 1972; Hendry et al. 1974; quoted, Mill 1982);

$k < 2 \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with singlet oxygen at 25°C in aquatic systems with $t_{1/2} > 100 \text{ yr}$ (Foote 1976; Mill 1979; quoted, Mill 1982);

aqueous photooxidation $t_{1/2} = 0.39\text{--}19.3 \text{ h}$ in surface water, based on measured rate data for the reaction with alkyl peroxy radical in aqueous solution (Mill 1982; selected, Howard et al. 1991);

photooxidation $t_{1/2} = 6\text{--}26.1 \text{ h}$ in air, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Atkinson 1987; selected, Howard et al. 1991);

72.1 mg/L of total organic carbon (TOC) degraded to 98% TOC after 5 h of illumination with a 250 W tungsten lamp by photo-Fenton reaction (Ruppert et al. 1993).

Hydrolysis: no hydrolyzable group (Howard et al. 1991).

Biodegradation: 95% degradation in 1–2 d in mixed bacteria cultures (Tabak et al. 1964);

average rate of biodegradation $54.2 \text{ mg COD g}^{-1}\cdot\text{h}^{-1}$ based on measurements of COD decrease using activated sludge inoculum with 20 d of adaptation to the substrate (Pitter 1976; quoted, Scow 1982);

aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on aqueous screening test data (Ludzack & Ettinger 1960; Belly & Goodhue 1976; Gerike & Fischer 1979; selected, Howard et al. 1991);

aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environmental Compartments:

Air: photooxidation $t_{1/2} = 6\text{--}26.1$ h, based on estimated rate constant for the vapor-phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

Surface water: aqueous photooxidation $t_{1/2} = 0.39\text{--}19.3$ h, based on measured rate data for the reaction with alkylperoxyl radical in aqueous solution (Mill 1982; quoted, Howard et al. 1991).

Ground water: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 14.1.4.7.1

Reported vapor pressures of hydroquinone (1,4-dihydroxybenzene) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log (P/\text{mmHg}) = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log (P/\text{Pa}) = A - B/(C + T/K)$		(3)			
$\log (P/\text{mmHg}) = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Vonderres et al. 1955		Bender et al. 1983	
summary of literature data		ebulliometry		gas saturation-IR	
t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa	t/ $^{\circ}\text{C}$	P/Pa
					solid
132.4	133.3*	159.1	1333	67.85	0.46
153.3	666.6*	181.0	3333	79.95	1.70
163.5	1333*	199.1	6666	90.75	4.79
174.6	2666	210.0	9999	100.75	11.2
192.0	5333	218.5	13332	111.25	26.9
203.0	7999	230.1	19998	116.05	40.2
216.5	13332	239.2	26664	121.15	61.1
238.0	26664	246.1	33330	126.45	92.3
262.5	53329	252.0	39997		
286.2	101325	254.8	43330	eq. 1a	P ^s /Pa
		257.2	46663	A	35.137
	*solid	259.0	53329	B	12233
mp/ $^{\circ}\text{C}$	170.3	266.1	59995		
		269.5	66661		
		273.0	73327		
		276.7	79993		
		278.8	86659		
		282.0	93325		
		286.0	101325		
		bp/ $^{\circ}\text{C}$	276.17		

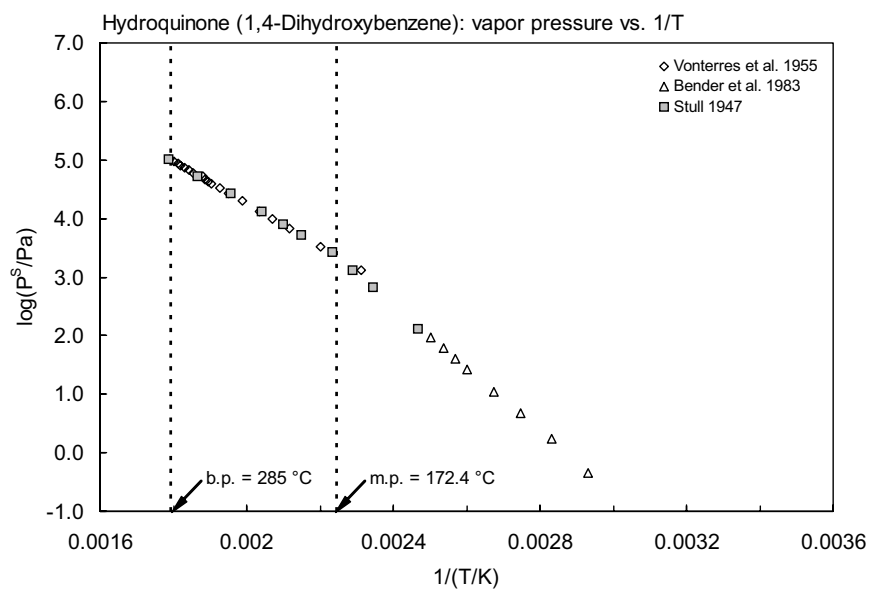
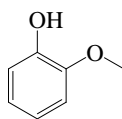


FIGURE 14.1.4.7.1 Logarithm of vapor pressure versus reciprocal temperature for hydroquinone.

14.1.4.8 2-Methoxyphenol (Guaiacol)



Common Name: Guaiacol

Synonym: 2-methoxyphenol, methylcatechol, *o*-hydroxyanisole, 1-hydroxy-2-methoxybenzene, pyrocatechol mono-methylether

Chemical Name: *o*-methoxyphenol

CAS Registry No: 90-05-1

Molecular Formula: $C_7H_8O_2$, $C_6H_4(OCH_3)OH$

Molecular Weight: 124.138

Melting Point ($^{\circ}C$):

32 (Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$): 204–206

205 (Lide 2003)

Density (g/cm^3):

1.129 (crystal)

1.112 (liquid, solidified at $28^{\circ}C$)

Acid Dissociation Constant, pK :

Molar Volume (cm^3/mol):

134.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 5 J/mol K$), F : 0.854 (mp at $32^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

143000–16700 (Windholz 1983)

16000 ($15^{\circ}C$, Verschueren 1983)

15000 (room temp., Dean 1985)

18700, 1316 ($15^{\circ}C$, $37^{\circ}C$, Yalkowsky et al. 1987)

24800 ($25^{\circ}C$, shake flask-HPLC/UV, Tam et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

133.3* ($52.4^{\circ}C$, summary of literature data, temp range 52.4 – $205^{\circ}C$, Stull 1947)

1333* ($82.0^{\circ}C$, ebulliometry, measured range 82.0 – $205.0^{\circ}C$, Vonterres et al. 1955)

$\log(P/mmHg) = [-0.2185 \times 13425.8/(T/K)] + 9.027299$; temp range 52.4 – $205^{\circ}C$ (Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [1 - 477.010/(T/K)] \times 10^4 \{0.858892 - 4.47192 \times 10^{-4} \cdot (T/K) + 3.228549 \times 10^{-7} \cdot (T/K)^2\}$; temp range 355.15 – $478.15 K$ (Cox eq., Chao et al. 1983)

13.73 (Verschueren 1983)

8.88 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.40415 - 1121.391/(125.407 + t/^{\circ}C)$; temp range 82 – $205^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

6.79 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.161 - 1051/(116.0 + t/^{\circ}C)$; temp range 82 – $205^{\circ}C$ (Antoine eq., Dean 1985, 1992)

24.5 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.44572 - 1786.15/(-76.43 + T/K)$; temp range 378 – $479 K$ (Antoine eq., Stephenson & Malanowski 1987)

21.00 (quoted, Sagebiel & Seiber 1993)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.30 (calculated-P/C, Sagebiel et al. 1992)

0.13, 0.11 (gas stripping-UV, headspace-GC, Sagebiel et al. 1992)
 0.132 (bubble chamber, Sagebiel & Seiber 1993)
 0.049 (calculated-group contribution, Lee et al. 2000)
 0.0724 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 6.198 - 3144/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.33 (shake flask-UV, Umeyama et al. 1971)
 1.35 (shake flask-UV, Korenman 1973)
 1.33 (shake flask-UV, Norrington et al. 1975)
 1.58 (Hansch & Leo 1979)
 1.25 (HPLC-RT correlation, Butte et al. 1981)
 1.32 (shake flask, Log P Database, Hansch & Leo 1987)
 1.32 (recommended, LOGKOW databank, Sangster 1993)
 1.32 (recommended, Hansch et al. 1995;)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

1.56 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.4.8.1
Reported vapor pressures of 2-methoxyphenol (guaiacol) at various temperatures

Stull 1947		Vonderres et al. 1955	
summary of literature data		ebulliometry	
t/°C	P/Pa	t/°C	P/Pa
52.4	133.3	82.0	1333
79.1	666.6	102.0	3333
92.0	1333	119.0	6666
106.0	2666	129.5	9999
121.6	5333	136.0	13332
131.0	7999	149.0	19998
144.0	13332	155.5	26664
162.7	26664	164.8	33330
184.1	53329	169.0	39997
205.0	101325	173.0	43330
		175.9	46663
mp/°C	28.5	179.0	53329
		184.7	59995
		187.0	66661
		191.0	73327
		194.0	79993
		198.0	86659
		201.0	93325
		205.0	101325
		bp/°C	204.566

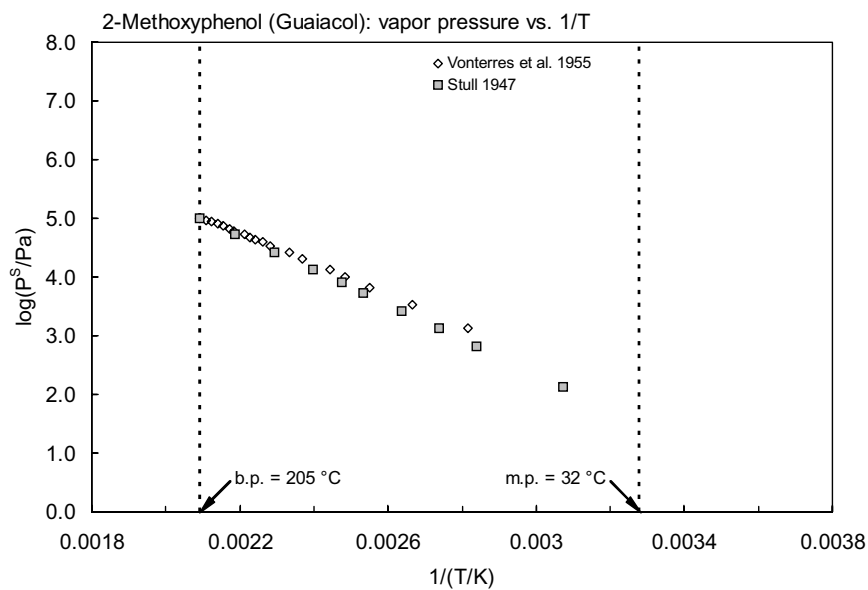
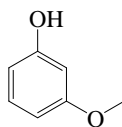


FIGURE 14.1.4.8.1 Logarithm of vapor pressure versus reciprocal temperature for 2-methoxyphenol (guaiacol).

14.1.4.9 3-Methoxyphenol



Common Name: 3-Methoxyphenol

Synonym: *m*-methoxyphenol, *m*-hydroxyanisole, resorcinol monomethylether

Chemical Name: 3-methoxyphenol

CAS Registry No: 150-19-6

Molecular Formula: $\text{CH}_3\text{OC}_6\text{H}_4\text{OH}$

Molecular Weight: 124.138

Melting Point ($^{\circ}\text{C}$):

< -17 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

244 (Stephenson & Malanowski 1987)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

134.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$), F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C):

67800 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.262 (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.12536 - 1572.51/(-136.16 + T/\text{K})$; temp range 413–518 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.10 (estimated as per Sagebiel et al. 1992 data on 2-methoxyphenol)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

1.58 (Leo et al. 1969; Hansch & Leo 1979)

1.47 (HPLC- k' correlation, Minick et al. 1988)

1.58 (COMPUTOX databank, Kaiser 1993)

1.58 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

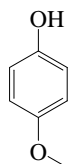
Sorption Partition Coefficient, $\log K_{\text{OC}}$:

1.50 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.10 4-Methoxyphenol



Common Name: 4-Methoxyphenol

Synonym: *p*-methoxyphenol, *p*-hydroxyanisole, hydroquinone monomethylether

Chemical Name: 4-methoxyphenol

CAS Registry No: 150-76-5

Molecular Formula: $\text{CH}_3\text{OC}_6\text{H}_4\text{OH}$

Molecular Weight: 124.138

Melting Point ($^{\circ}\text{C}$):

57 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

243 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

134.7 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$, F: 0.485 (mp at 57°C))

Water Solubility (g/m^3 or mg/L at 25°C):

40000 (Verschueren 1977, 1983)

19500 (shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

0.033 (extrapolated-Antoine eq., Boublik et al. 1984)

0.556 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_g/\text{kPa}) = 12.27865 - 4631.266/(T/\text{K})$; temp range 278–300 K (Antoine eq.-I, solid, Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 6.8462 - 2111.03/(-81.56 + T/\text{K})$; temp range 418–518 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

0.979 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/\text{Pa}) = -3664/(T/\text{K}) + 12.28$ (GC-RT correlation, Lei et al. 1999)

1.05 (supercooled liquid P_L , calculated-group contribution, Lee et al. 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

Octanol/Water Partition Coefficient, $\log K_{\text{ow}}$:

1.34 (shake flask-UV, Fujita et al. 1964)

1.37 (shake flask-UV at pH 7.45, Umeyama et al. 1971)

1.34, 1.33, 1.37 (lit. values, Hansch & Leo 1979)

1.47 (shake flask, Korenman et al. 1980)

1.62 (HPLC- k' correlation, Miyake & Terada 1982)

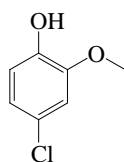
1.24 (HPLC- k correlation, Minick et al. 1988)

1.34 (recommended, LOGKOW databank, Sangster 1993)

1.34 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{oc}}$:

14.1.4.11 4-Chloroguaiacol

Common Name: 4-Chloroguaiacol

Synonym: 4-chloromethoxyphenol

Chemical Name: 4-chloroguaiacol, 4-chloromethoxyphenol

CAS Registry No: 16766-30-6

Molecular Formula: $C_7H_7ClO_2$

Molecular Weight: 158.582

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

155.6(calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol·K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

5140 (shake flask-HPLC/UV, pH 2.8, Tam et al. 1994)

5604 (shake flask-GC/ECD, pH 2.8, Tam et al. 1994)

5370 (selected, Tam et al. 1994)

4856* ($19^{\circ}C$, shake flask-HPLC/UV, measured range 10 – $50^{\circ}C$, Larachi et al. 2000)

5132; 13200, 10500 (quoted exptl.; calculated-group contribution, calculated-AQAUFAC, Lee et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.15 (calculated-fragment const., Niimi et al. 1990)

2.11–2.52 (literature range, NCASI 1992)

Bioconcentration Factor, $\log BCF$:

0.0 (trout, 1–21 d exposure, $BCF < 1$, Niimi et al. 1990)

0.86–1.19 (quoted, NCASI 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

TABLE 14.1.4.11.1

Reported aqueous solubilities of 4-chloroguaiacol at various temperatures

Larachi et al. 2000

shake flask-HPLC/UV

t/°C	S/g·m ⁻³
10.0	4395
11.0	4467
15.0	4548
19.0	4856
36.3	5406
41.0	6658
50.0	6213
54.5	7054
66.0	7040
70.5	8639
78.0	9171
85.6	9540
90.0	10255

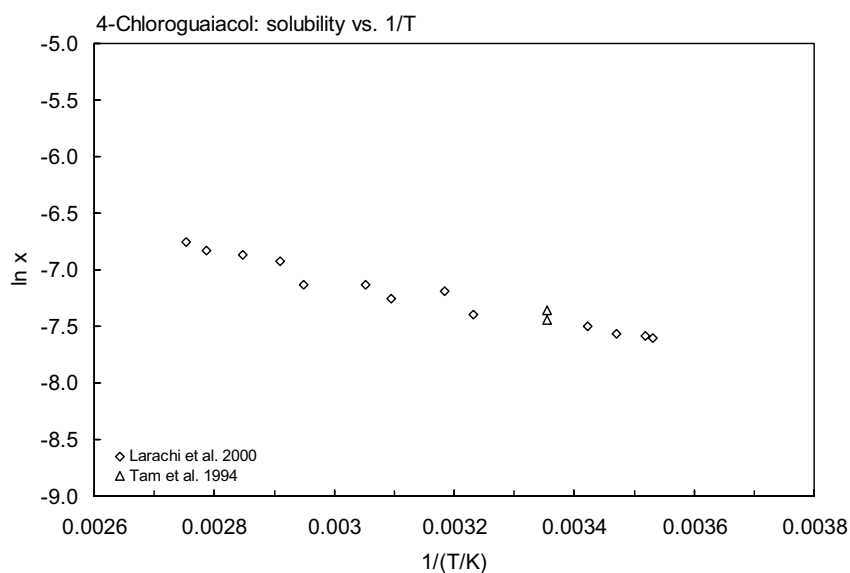
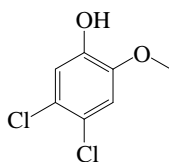


FIGURE 14.1.4.11.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 4-chloroguaiacol.

14.1.4.12 4,5-Dichloroguaiacol



Common Name: 4,5-Dichloroguaiacol

Synonym: 4,5-dichloro-2-methoxyphenol

Chemical Name: 4,5-dichloroguaiacol

CAS Registry No: 2460-49-3

Molecular Formula: $C_7H_6Cl_2O_2$

Molecular Weight: 193.028

Melting Point ($^{\circ}C$): 69–70

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

8.26, 8.52 (20 $^{\circ}C$, regressions, Xie & Dyrssen 1984)

Molar Volume (cm^3/mol):

176.5 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at 25 $^{\circ}C$):

584 (shake flask-HPLC/UV, pH 5.6, Tam et al. 1994)

565 (shake flask-GC/ECD, pH 5.6, Tam et al. 1994)

3130, 1086 (supercooled liquid values: calculated-group contribution, calculated- AQUAFAC, Lee et al. 2000)

Vapor Pressure (Pa at 25 $^{\circ}C$):

1.54 (supercooled liquid P_L , correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa\cdot m^3/mol$ at 25 $^{\circ}C$):

0.44 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.04 (calculated-fragment const., Rekker 1977)

3.28 (Hansch & Leo 1979)

3.26 (shake flask-UV, Saarikoski & Viluksela 1982)

3.18 (shake flask-GC, Xie et al. 1984)

3.28 (HPLC- k' correlation, Xie et al. 1984)

3.20, 3.19, 3.19 (shake flask-GC, regressions, Xie & Dryssen 1984)

3.26 (recommended, Sangster 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.74–2.05, 2.03 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)

1.18–1.51, 1.75 (quoted, estimated, NCASI 1992)

2.03 (*Oncorhynchus mykiss*, quoted, Devillers et al. 1996)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

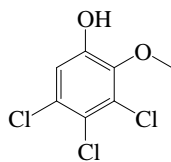
Biodegradation: 5% reduction in concn (5 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d (Neilson et al. 1991)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

14.1.4.13 3,4,5-Trichloroguaiacol



Common Name: 3,4,5-Trichloroguaiacol

Synonym: 3,4,5-trichloro-2-methoxyphenol

Chemical Name: 3,4,5-trichloroguaiacol

CAS Registry No: 57057-83-7

Molecular Formula: $C_7H_3Cl_3O_2$

Molecular Weight: 227.473

Melting Point ($^{\circ}C$): 85–86

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.55 (Könemann 1981)

7.43, 7.52, 7.56 ($20^{\circ}C$, regressions, Xie & Dyrssen 1984)

7.90 (Leuenberger et al. 1985)

7.56 (Xie et al. 1986)

Molar Volume (cm^3/mol):

197.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

305 (shake flask-HPLC/UV, pH 5.9, Tam et al. 1994)

313 (shake flask-GC/ECD, pH 5.9, Tam et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

0.64 (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.12 (calculated-P/C, Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.77 (shake flask-UV, Saarikoski & Viluksela 1982)

4.11 (shake flask-GC, Xie et al. 1984)

4.18 (HPLC- k' correlation, Xie et al. 1984)

4.14 (shake flask-GC, Xie & Dyrssen 1984)

3.77 (recommended, Sangster 1993)

3.77 (COMPUTOX databank, Kaiser 1993)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.60 (rainbow trout, Oikari et al. 1985)

2.06–2.51, 2.41 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)

1.78–1.95 (field studies, bile of rainbow trout, Niimi et al. 1990)

2.47 (estimated, NCASI 1992)

2.20 (*Oncorhynchus mykiss*, Devillers et al. 1996)

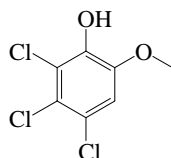
Sorption coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

Biota: $t_{1/2} = 1\text{--}2$ d in bleak and $t_{1/2} = 2$ d in trout (Niimi et al. 1990).

14.1.4.14 4,5,6-Trichloroguaiacol



Common Name: 4,5,6-Trichloroguaiacol

Synonym: 2,3,4-trichloro-6-methoxyphenol

Chemical Name: 4,5,6-trichloroguaiacol

CAS Registry No: 2668-24-8

Molecular Formula: $C_7H_5Cl_3O_2$

Molecular Weight: 227.473

Melting Point ($^{\circ}C$): 112–115

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.07 (Leuenberger et al. 1985)

7.20 ($20^{\circ}C$, regressions, Xie & Dyrssen 1984)

Molar Volume (cm^3/mol):

197.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

57.0 (shake flask-HPLC/UV, pH 5.8, Tam et al. 1994)

50.0 (shake flask-GC/ECD, pH 5.8, Tam et al. 1994)

Vapor Pressure (Pa at $25^{\circ}C$):

0.249 (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

8.82 (calculated-P/C)

0.14 (calculated-P/C, Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.74 (shake flask-GC, Xie et al. 1984)

3.92, 3.91, 3.78 (HPLC- k' correlation, calculated- π const., calculated- f const., Xie et al. 1984)

3.73, 3.74, 3.72 (shake flask-GC, regressions, Xie & Dyrssen 1984)

3.57 (calculated-fragment const., Niimi et al. 1990)

3.72, 3.92 (literature values, Sangster 1993)

3.82 (COMPUTOX databank, Kaiser 1993)

3.72, 3.92 (literature values, Hansch et al. 1995)

3.19 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.60 (bleaks, Renberg et al. 1980)

1.90–2.11 (rainbow trout, Oikari et al. 1985)

2.59 (bleaks, Walden et al. 1986)

- 1.88–2.05, 1.97 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
1.78–1.95 (field studies, bile of trout, Niimi et al. 1990)
4.81 (fourhorn sculpin *myoxocephalus quadricornis*, bile BCF in brackish water, during 6–20 d exposure under continuous water-flow conditions, Wachtmeister et al. 1991)
2.22 (estimated, NCASI 1992)
1.97 (*Oncorhynchus mykiss*, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{oc} :

- 3.11 (sediment, $K_p = 1.3 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986, quoted, Neilson et al. 1991)
2.80, 2.94 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.80 (soil, calculated-MCI $^1\chi$, Sabljic et al. 1995)
1.35 (sediment, $K_p = 22 \text{ ml kg of organic C}^{-1}$, batch sorption equilibrium, Remberger et al. 1986; Neilson et al. 1991)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: 16% reduction in concn (5 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

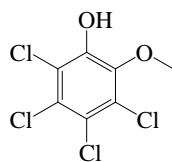
Biotransformation:

Bioconcentration, Uptake(k_1) and Elimination (k_2) Rate Constants Rates:

Half-Lives in the Environment:

Biota: $t_{1/2} = 1$ to 2 d in bleak (Niimi et al. 1990).

14.1.4.15 3,4,5,6-Tetrachloroguaiacol



Common Name: 3,4,5,6-Tetrachloroguaiacol

Synonym: 2,3,4,5-tetrachloro-6-methoxyphenol

Chemical Name: 3,4,5,6-tetrachloroguaiacol

CAS Registry No: 2539-17-5

Molecular Formula: $C_7H_4Cl_4O_2$

Molecular Weight: 261.918

Melting Point ($^{\circ}C$): 121–122

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.26 (Leuenberger et al. 1985)

6.19, 6.12, 6.26 ($20^{\circ}C$, regressions, Xie & Dyrssen 1984)

Molar Volume (cm^3/mol):

218.3 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

27.0 (shake flask-HPLC/UV, pH 4.2, Tam et al. 1994)

25.0 (shake flask-GC/ECD, pH 4.2, Tam et al. 1994)

165, 28 (supercooled liquid values: calculated-group contribution, calculated-AQAUFAC, Lee et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

0.138 (supercooled liquid value, correlated-GC-RT, Bidleman & Renberg 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

1.013 (Leuenberger et al. 1985; quoted, Barton 1987)

0.15 (calculated-P/C, Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.29 (Saarikoski & Viluksela 1982)

4.45 (shake flask-GC, Xie et al. 1984)

4.76, 5.01, 4.52 (HPLC- k' correlation, calculated- π const., calculated-fragment const., Xie et al. 1984)

4.41, 4.43, 4.42 (shake flask, regressions, Xie & Dyrssen 1984)

4.53 (Leuenberger et al. 1985)

4.28 (calculated-fragment, Niimi et al. 1990)

4.59 (COMPUTOX databank, Kaiser 1993)

4.42, 4.76 (literature values, Sangster 1993)

4.42 (selected, Hansch et al. 1995)

3.83 (from Panoma database or calculated from MedChem program, Sabljic et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.60 (bleaks, after 2 weeks exposure, Renberg et al. 1980)

1.60–2.18 (rainbow trout, Oikari et al. 1985)

- 1.78–1.95 (bile of rainbow trout, field studies, Niimi et al. 1990)
2.04–2.38, 2.26 (rainbow trout: 1–21 d exposure, mean value, Niimi et al. 1990)
3.20 (roach, Niimi et al. 1990, quoted, NCASI 1992)
2.84 (estimated, NCASI 1992)
2.26 (*Oncorhynchus mykiss*, Devillers et al. 1996)

Sorption Partition Coefficient, log K_{OC} :

- 2.85 (soil, Seip et al. 1986)
3.15 (sediment, $K_p = 1.5 \text{ ml} \cdot (\text{kg of organic C})^{-1}$, batch sorption equilibrium, Remberger et al. 1986)
2.30 (soil, calculated-MCI χ , Bahnick & Doucette 1988)
2.85, 3.17 (soil, quoted, calculated-MCI χ and fragment contribution, Meylan et al. 1992)
2.85 (soil, calculated-MCI χ , Sabljic et al. 1995)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: 100% reduction in concn (5 -M) after incubation with cells of *Rhodococcus chlorophenolicus* for 14 d under aerobic conditions (Neilson et al. 1991)

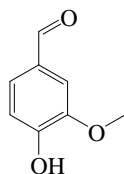
Biotransformation:

Bioconcentration, Uptake(k_1) and Elimination (k_2) Rate Constants Rates:

Half-Lives in the Environment:

Biota: $t_{1/2} < 10$ d in trout liver (Niimi et al. 1990); $t_{1/2} = 1\text{--}2$ d in bleak (Niimi et al. 1990).

14.1.4.16 Vanillin (4-Hydroxy-3-methoxybenzaldehyde)



Common Name: Vanillin

Synonym: 4-hydroxy-3-methoxybenzaldehyde, vanillic aldehyde, methylprotocatechuic aldehyde

Chemical Name: 4-hydroxy-3-methoxybenzaldehyde

CAS Registry No: 121-33-5

Molecular Formula: $C_8H_8O_3$, $C_6H_3OHCHO(OCH_3)$

Molecular Weight: 152.148

Melting Point ($^{\circ}C$):

81.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

285 (Weast 1982–83; Lide 2003)

284 (decomposes, Stephenson & Malanowski 1987)

Density (g/cm^3):

1.056 (Weast 1982–83)

Acid Dissociation Constant, pK_a :

7.40 (Sangster 1993)

7.62 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

156.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.279 (mp at $81.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2480 (at pH 4.50, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

133.3 ($107^{\circ}C$, summary of literature data, temp range 107 – $285^{\circ}C$, Stull 1947)

$\log(P_S/kPa) = 10.997 - 4623/(T/K)$; temp range 288 – 333 K (solid, Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_S/kPa) = 10.93562 - 4535.023/(T/K)$; temp range 297 – 328 K (solid, Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 7.01734 - 3198.18/(-17.047 + T/K)$; temp range 380 – 558 K (Antoine eq.-III, Stephenson & Malanowski 1987)

$\log(P/mmHg) = -25.583 - 4.086 \times 10^3/(T/K) + 17.515 \cdot \log(T/K) - 2.8177 \times 10^{-2} \cdot (T/K) + 1.0912 \times 10^{-5} \cdot (T/K)^2$; temp range 355 – 777 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.31 (shake flask-UV, Korenman & Sotnikova 1975)

1.21 (shake flask-UV, Holmes & Lough 1976)

1.21 (shake flask-HPLC, Bazaco & Coca 1989)

1.21 (recommended, Sangster 1993)

1.21 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

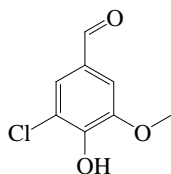
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.17 5-Chlorovanillin



Common Name: 5-Chlorovanillin

Synonym:

Chemical Name: 5-chlorovanillin

CAS Registry No: 19463-48-0

Molecular Formula: $C_8H_7ClO_3$, $C_6H_2ClCHO(OCH_3)$

Molecular Weight: 185.593

Melting Point ($^{\circ}C$):

165 (Weast 1982–83; Lide 2003)

169 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a

6.80 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

177.8 (Le Bas method -calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.042 (mp at $165^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

932 (at pH 4.55, shake flask-HPLC/UV, Varhaníčková et al 1995)

249* ($24^{\circ}C$, shake flask-HPLC/UV, measured range 7.5 – $85.9^{\circ}C$, Larachi et al. 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.76 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

0.59 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

TABLE 14.1.4.17.1

Reported aqueous solubilities of 5-chlorovanillin at various temperatures

Larachi et al. 2000

shake flask-HPLC/UV	
t/°C	S/g·m ⁻³
7.5	171
12.0	171
16.8	184
19.8	168
24.0	249
30.0	286
36.5	505
46.0	629
50.0	760
59.0	932
65.0	1139
70.0	1267
80.0	1767
85.9	2314

$\Delta S_{\text{fus}}/(\text{kJ mol}^{-1}) = 89.1$

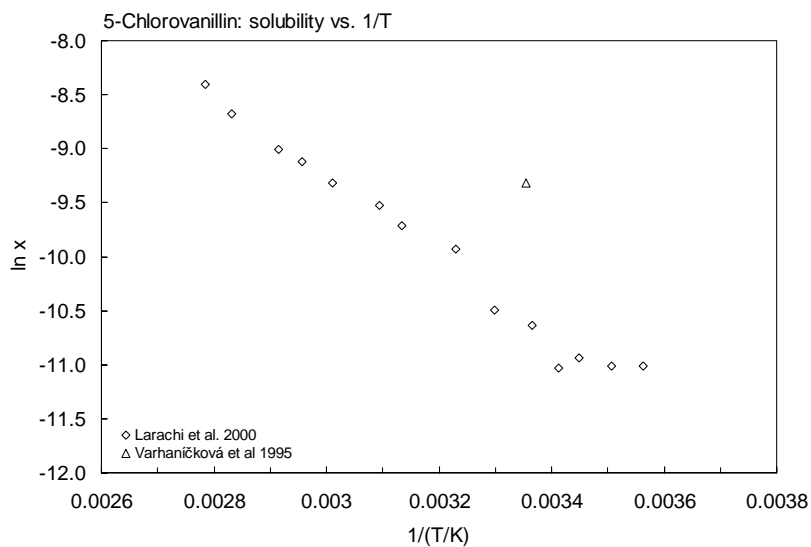
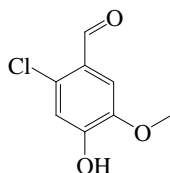


FIGURE 14.1.4.17.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for 5-chlorovanillin.

14.1.4.18 6-Chlorovanillin



Common Name: 6-Chlorovanillin

Synonym:

Chemical Name: 6-chlorovanillin

CAS Registry No: 18268-76-3

Molecular Formula: $C_8H_7ClO_3$, $C_6H_2ClCHO(OCH_3)$

Molecular Weight: 185.593

Melting Point ($^{\circ}C$):

171–172 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.11 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

177.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

132 (at pH 5.35, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.76 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{oa}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

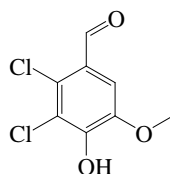
0.59 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.19 5,6-Dichlorovanillin



Common Name: 5,6-Dichlorovanillin

Synonym:

Chemical Name: 5,6-dichlorovanillin

CAS Registry No: 18268-69-4

Molecular Formula: $C_8H_6Cl_2O_3$, $C_6HCl_2CHO(OCH_3)$

Molecular Weight: 221.038

Melting Point ($^{\circ}C$):

198–199 (Varhanířková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

5.28 (Varhanířková et al 1995)

Molar Volume (cm^3/mol):

198.7 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

23.0 (at pH 4.0, shake flask-HPLC/UV, Varhanířková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa\ m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.47 (NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{oa}$:

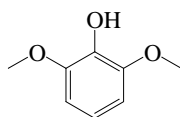
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.76 (estimated, K_{ow} , NCASI 1996)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.20 Syringol (2,6-Dimethoxyphenol)

Common Name: Syringol

Synonym: 2,6-dimethoxyphenol

Chemical Name: 2,6-dimethoxyphenol

CAS Registry No: 91-10-1

Molecular Formula: C₈H₁₀O₃, C₆H₃OH(OCH₃)₂

Molecular Weight: 154.163

Melting Point (°C):

53–56 (Aldrich catalog 1998–1999)

56.5 (Lide 2003)

Boiling Point (°C):

261 (Aldrich catalog 1998–1999; Lide 2003)

Density (g/cm³):

Acid Dissociation Constant, pK_a:

Molar Volume (cm³/mol):

166.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

18200 (shake flask-UV spectroscopy, Sagebiel & Seiber 1993)

Vapor Pressure (Pa at 25°C):

0.45 (GC-RT correlation, Sagebiel & Seiber 1993)

Henry's Law Constant (Pa m³/mol at 25°C):

0.00271 (gas stripping-GC, Sagebiel & Seiber 1993)

Octanol/Water Partition Coefficient, log K_{ow}:

1.15 (shake flask-UV, Fujita et al. 1964)

1.15 (recommended, Sangster 1993)

1.15 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, log K_{oa}:

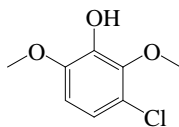
Bioconcentration Factor, log BCF or log K_B:

Sorption Partition Coefficient, log K_{oc}:

Environmental Fate Rate Constants, k, and Half-Lives, t_{1/2}:

Half-Lives in the Environment:

14.1.4.21 3-Chlorosyringol



Common Name: 3-Chlorosyringol

Synonym: 3-chloro-2,6-dimethoxyphenol

Chemical Name: 3-chlorosyringol

CAS Registry No: 18113-22-9

Molecular Formula: $C_8H_9ClO_3$, $C_6H_2(OH)Cl(OCH_3)_2$

Molecular Weight: 188.608

Melting Point ($^{\circ}C$):

35-36 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

9.09 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

186.9 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

68.6 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

5170 (at pH 4.30, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.825 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3580/(T/K) - 11.93$ (GC-RT correlation, Lei et al. 2001)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.011 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

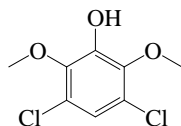
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.22 3,5-Dichlorosyringol



Common Name: 3,5-Dichlorosyringol

Synonym: 3,5-dichloro-2,6-dimethoxyphenol

Chemical Name: 3,5-dichlorosyringol

CAS Registry No: 78782-46-4

Molecular Formula: $C_8H_8Cl_2O_2$, $C_6H(OH)Cl_2(OCH_3)_2$

Molecular Weight: 223.054

Melting Point ($^{\circ}C$):

105–106 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constants, pK_a :

7.27 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

207.8 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

70.4 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

244 (at pH 5.80, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.465 (supercooled liquid P_L , GC-RT correlation, Lei et al. 1999)

$\log(P_L/Pa) = -3679/(T/K) - 12.01$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.069 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

Octanol/Air Partition Coefficient, $\log K_{OA}$:

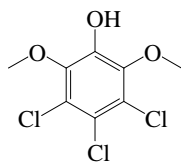
Bioconcentration Factor, $\log BCF$ or $\log K_B$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.23 Trichlorosyringol



Common Name: Trichlorosyringol

Synonym: 3,4,5-trichloro-2,6-dimethoxyphenol

Chemical Name: 3,4,5-trichloro-2,6-dimethoxyphenol

CAS Registry No: 2539-26-6

Molecular Formula: $C_8H_7Cl_3O_3$, $C_6(OH)Cl_3(OCH_3)_2$

Molecular Weight: 257.499

Melting Point ($^{\circ}C$):

122–123 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

7.73 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

228.7 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.4 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

100 (at pH 3.90, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.077 (supercooled liquid P_L , GC-RT correlation; Lei et al. 1999)

$\log(P_L/Pa) = -4014/(T/K) - 12.44$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.022 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.74 (shake flask-GC, Saarikoski & Viluksela 1982)

4.20 (quoted, NCASI 1992)

3.74 (recommended, Sangster 1993)

3.74 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

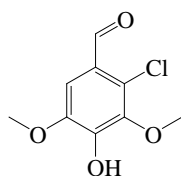
1.19 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.24 2-Chlorosyringaldehyde



Common Name: 2-Chlorosyringaldehyde

Synonym:

Chemical Name: 2-chlorosyringaldehyde

CAS Registry No: 76341-69-0

Molecular Formula: $C_9H_9ClO_4$, $C_6H(OH)Cl(CHO)(OCH_3)_2$

Molecular Weight: 216.619

Melting Point ($^{\circ}C$):

196–197 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

6.80 (Varhaníčková et al 1995)

Molar Volume (cm^3/mol):

209.1 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

77.7 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

33 (at pH 5.30, shake flask-HPLC/UV, Varhaníčková et al 1995)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.079 (supercooled liquid P_L , GC-RT correlation; Lei et al. 1999)

$\log(P_L/Pa) = -4058/(T/K) - 12.51$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.069 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.81 (quoted, NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

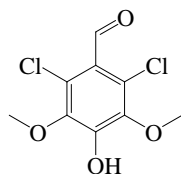
0.62 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.1.4.25 2,6-Dichlorosyringaldehyde



Common Name: 2,6-Dichlorosyringaldehyde

Synonym:

Chemical Name:

CAS Registry No: 76330-06-8

Molecular Formula: $C_9H_8Cl_2O_4$, $C_6(OH)Cl_2(CHO)(OCH_3)_2$

Molecular Weight: 251.064

Melting Point ($^{\circ}C$):

195.6 (Varhaníčková et al 1995)

Boiling Point ($^{\circ}C$):

Density (g/cm^3):

Acid Dissociation Constant, pK_a :

Molar Volume (cm^3/mol):

230.0 (Le Bas method-calculated at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

82.2 (Lei et al. 1999)

Enthalpy of Sublimation, ΔH_{subl} (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

26.0 (at pH 4.60, shake flask-HPLC/UV, Varhaníčková et al. 1995)

Vapor Pressure (Pa at $25^{\circ}C$):

0.025 (supercooled liquid P_L , GC-RT correlation; Lei et al. 1999)

$\log(P_L/Pa) = -4293/(T/K) - 12.79$, (GC-RT correlation, Lei et al. 1999)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.0037 (calculated- P_L/C_L , Lei et al. 1999)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.52 (quoted, NCASI 1992)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

1.19 (estimated- K_{ow} , NCASI 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

14.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 14.2.1

Summary of physical properties of phenolic compounds

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a
							MW/ ρ at 20°C	Le Bas	
Alkylphenols and other substituted phenols:									
Phenol	108-95-2	C ₆ H ₅ OH	94.111	40.89	181.87	0.698	88.99	103.4	9.89
<i>o</i> -Cresol (2-Methylphenol)	95-48-7	C ₆ H ₄ (CH ₃)OH	108.138	31.03	191.04	0.873	105.26	125.6	10.26
<i>m</i> -Cresol (3-Methylphenol)	108-39-4	C ₆ H ₄ (CH ₃)OH	108.138	12.24	202.27	1	104.62	125.6	10
<i>p</i> -Cresol (4-Methylphenol)	106-44-5	C ₆ H ₄ (CH ₃)OH	108.138	34.77	201.98	0.802	106.25	125.6	10.26
2,6-Di- <i>t</i> -butyl-4-methylphenol	128-37-0	C ₁₅ H ₂₄ O	220.351	71	265	0.354		303.2	
2,3-Dimethylphenol	526-75-0	C ₈ H ₁₀ O	122.164	72.5	216.9	0.342		147.8	
2,4-Dimethylphenol	105-67-9	C ₈ H ₁₀ O	122.164	24.5	210.98	1		147.8	10.6
2,5-Dimethylphenol	98-87-4	C ₈ H ₁₀ O	122.164	74.8	211.1	0.325		147.8	10.3
2,6-Dimethylphenol	576-26-1	C ₈ H ₁₀ O	122.164	45.8	201.07	0.625		147.8	10.6
3,4-Dimethylphenol	95-65-8	C ₈ H ₁₀ O	122.164	65.1	227	0.404	124.28	147.8	10.4
3,5-Dimethylphenol	108-68-9	C ₈ H ₁₀ O	122.164	63.4	221.74	0.420		147.8	10.2
2,3,5-Trimethylphenol	697-82-5	C ₉ H ₁₂ O	136.190	94.5	233	0.208		170.0	10.6
2,3,6-Trimethylphenol	2416-94-6	C ₉ H ₁₂ O	136.190	63		0.424		170.0	
2,4,5-Trimethylphenol	496-78-6	C ₉ H ₁₂ O	136.190	72	232	0.346		170.0	
2,4,6-Trimethylphenol	527-60-6	C ₉ H ₁₂ O	136.190	73	220	0.338		170.0	10.9
3,4,5-Trimethylphenol	527-54-8	C ₉ H ₁₂ O	136.190	108	248.5	0.153		170.0	
3-Methyl-5-ethylphenol		C ₉ H ₁₂ O	136.190					170.0	10.1
<i>o</i> -Ethylphenol	90-00-6	C ₈ H ₁₀ O	122.164	18	204.5	1		147.8	
<i>m</i> -Ethylphenol	620-17-7	C ₈ H ₁₀ O	122.164	−4	218.4	1		147.8	
<i>p</i> -Ethylphenol	123-07-9	C ₈ H ₁₀ O	122.164	45	217.9	0.636		147.8	
2-Propylphenol	644-35-9	C ₉ H ₁₂ O	136.190	7	220	1		170.0	
4-Propylphenol	645-56-7	C ₉ H ₁₂ O	136.190	22	232.6	1	134.98	170.0	10.3
2-Isopropylpheonol	88-69-7	C ₉ H ₁₂ O	136.190	15.5	213.5	1		170.0	
4-Isopropylphenol	99–89–8	C ₉ H ₁₂ O	136.190	62.3	230	0.431		170.0	10.3
4-Butylphenol	1638-22-8	C ₁₀ H ₁₄ O	150.217	22	248	1		192.2	10.3
2- <i>sec</i> -Butylphenol	89–72–5	C ₁₀ H ₁₄ O	150.217	16	228	1		192.2	
2- <i>tert</i> -Butylphenol	88-18-6	C ₁₀ H ₁₄ O	150.217	B6.8	223	1		192.2	

(Continued)

TABLE 14.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M cm ³ /mol		pK _a
							MW/ ρ at 20°C	Le Bas	
3- <i>tert</i> -Butylphenol	585-34-2	C ₁₀ H ₁₄ O	150.217	42.3	240	0.676		192.2	10.1
4- <i>sec</i> -Butylphenol	99-71-8	C ₁₀ H ₁₄ O	150.217	61.5	241	0.438		192.2	
4- <i>tert</i> -Butylphenol	98-54-4	C ₁₀ H ₁₄ O	150.217	98	237	0.192		192.2	9.9
2-Methyl-5- <i>tert</i> -butylphenol		C ₁₁ H ₁₆ O	164.244					214.4	
2,6-Di- <i>sec</i> -butylphenol	128-39-2	C ₁₄ H ₂₂ O	206.324	39		0.729		281.0	
3,5-Di- <i>tert</i> -butylphenol	1138-52-9	C ₁₄ H ₂₂ O	206.323	88		0.241		281.0	
3-Pentylphenol		C ₁₁ H ₁₆ O	164.244					214.4	
4-Hexylphenol	2446-69-7	C ₁₂ H ₁₈ O	178.270	32		0.854		236.6	
2-Heptylphenol		C ₁₃ H ₂₀ O	192.297					258.8	
4-Heptylphenol	1987-50-4	C ₁₃ H ₂₀ O	192.297					258.8	
4-Octylphenol	1806-26-4	C ₁₄ H ₂₂ O	206.324	43		0.666		281.0	
4- <i>tert</i> -Octylphenol	140-66-9	C ₁₄ H ₂₂ O	206.324	85.8	279	0.253		281.0	
4-Nonylphenol	104-40-5	C ₁₅ H ₂₄ O	220.351	42	approx. 295	0.681		303.2	
1-Naphthol	90-15-3	C ₁₀ H ₈ O	144.170	95	288	0.206		155.0	
2-Naphthol	135-19-3	C ₁₀ H ₈ O	144.170	121.5	285	0.113	112.63	155.0	
2-Phenylphenol (2-Hydroxybiphenyl)	90-43-7	C ₁₂ H ₁₀ O	170.206	57.5	286	0.480		192.0	
3-Phenylphenol (3-Hydroxybiphenyl)	588-51-8	C ₁₂ H ₁₀ O	170.206	78	>300	0.302		192.0	
4-Phenylphenol (4-Hydroxybiphenyl)	92-69-3	C ₁₂ H ₁₀ O	170.206	166	305	0.0414		192.0	
2-Allylphenol	1745-81-9	C ₉ H ₁₀ O	134.174	B6	220	1		162.6	
Chlorophenols:									
2-Chlorophenol	95-57-8	C ₆ H ₄ OHCl	128.556	9.4	174.9	1	101.75	124.3	8.49
3-Chlorophenol	108-43-0	C ₆ H ₄ OHCl	128.556	32.6	214	0.842		124.3	8.85
4-Chlorophenol	106-48-9	C ₆ H ₄ OHCl	128.556	42.8	220	0.669	101.62	124.3	9.18
2,3-Dichlorophenol	576-24-9	C ₆ H ₄ Cl ₂ O	163.001	58	206	0.474		145.2	6.44
2,4-Dichlorophenol	120-83-2	C ₆ H ₄ Cl ₂ O	163.001	45	210	0.636		145.2	7.68
2,5-Dichlorophenol	583-78-8	C ₆ H ₄ Cl ₂ O	163.001	59	211	0.464		145.2	6.45
2,6-Dichlorophenol	87-65-0	C ₆ H ₄ Cl ₂ O	163.001	68.5	220	0.374		145.2	6.8
3,4-Dichlorophenol	95-77-2	C ₆ H ₄ Cl ₂ O	163.001	68	253	0.379		145.2	7.39
3,5-Dichlorophenol	591-35-5	C ₆ H ₄ Cl ₂ O	163.001	68	233	0.379		145.2	6.92
2,3,4-Trichlorophenol	15950-66-0	C ₆ H ₃ Cl ₃ O	197.446	83.5	sublim	0.267		166.1	7.66
2,3,5-Trichlorophenol	933-78-8	C ₆ H ₃ Cl ₃ O	197.446	62		0.433		166.1	7.37
2,3,6-Trichlorophenol	933-75-5	C ₆ H ₃ Cl ₃ O	197.446	58		0.474		166.1	7.13
2,4,5-Trichlorophenol	95-95-4	C ₆ H ₃ Cl ₃ O	197.446	69	247	0.370		166.1	7.43

2,4,6-Trichlorophenol	88-06-2	C ₆ H ₃ Cl ₃ O	197.446	69	246	0.370	166.1	7.42
3,4,5-Trichlorophenol	609-19-8	C ₆ H ₃ Cl ₃ O	197.446	101	275	0.180	166.1	7.74
2,3,4,5-Tetrachlorophenol	4901-51-3	C ₆ H ₂ Cl ₄ O	231.891	116.5	sublim	0.127	187.0	6.96
2,3,4,6-Tetrachlorophenol	58-90-3	C ₆ H ₂ Cl ₄ O	231.891	70		0.362	187.0	5.38
2,3,5,6-Tetrachlorophenol	935-95-5	C ₆ H ₂ Cl ₄ O	231.891	115		0.131	187.0	5.48
Pentachlorophenol	87-86-5	C ₆ HCl ₅ O	266.336	174	310 dec	0.0345	207.9	4.92
4-Chloro- <i>m</i> -cresol	59-50-7	C ₇ H ₇ ClO	142.583	67	235	0.387	146.5	
Nitrophenols:								
2-Nitrophenol	88-75-5	C ₆ H ₄ OHNO ₂	139.109	44.8	216	0.639	131.9	7.23
3-Nitrophenol	554-84-7	C ₆ H ₄ OHNO ₂	139.109	96.8		0.197	131.9	8.36
4-Nitrophenol	100-02-7	C ₆ H ₄ OHNO ₂	139.109	113.6	279	0.135	131.9	7.08
2,4-Dinitrophenol	51-28-5	C ₆ H ₄ N ₂ O ₅	184.106	114.8	sublim	0.132	160.4	4.09
2,6-Dinitrophenol	329-71-5	C ₆ H ₄ N ₂ O ₅	184.106	108		0.153	160.4	
2,4,6-Trinitrophenol (Picric acid)	88-89-1	C ₆ H ₃ N ₃ O ₇	229.104	122.5	300 exp	0.111	188.9	0.8
4,6-Dinitro- <i>o</i> -cresol	534-52-1	C ₇ H ₆ N ₂ O ₅	198.133	86.5		0.249	182.6	4.35
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:								
Catechol (1,2-Dihydroxybenzene)	120-80-9	C ₆ H ₄ (OH) ₂	110.111	104.6	245	0.166	110.8	9.5
3,5-Dichlorocatechol	13673-9-2	C ₆ H ₂ Cl ₂ (OH) ₂	179.001	83-84		0.267	152.6	7.78
4,5-Dichlorocatechol	3428-24-8	C ₆ H ₂ Cl ₂ (OH) ₂	179.001	116-117		0.127	152.6	
3,4,5-Trichlorocatechol	56961-20-7	C ₆ HCl ₃ (OH) ₂	213.446	134		0.0850	173.5	6.95
Tetrachlorocatechol	1198-55-6	C ₆ Cl ₄ (OH) ₂	247.891	194		0.0220	194.4	5.83
Resorcinol (1,3-Dihydroxybenzene)	108-46-3	C ₆ H ₄ (OH) ₂	110.111	109.4	276.5	0.149	110.8	9.4
Hydroquinone (1,4-Dihydroxybenzene)	123-31-9	C ₆ H ₄ (OH) ₂	110.111	172.4	285	0.0358	110.8	
2-Methoxyphenol (Guaiacol)	90-05-1	C ₇ H ₈ O ₂	124.138	32	205	0.854	134.7	
3-Methoxyphenol	150-19-6	C ₇ H ₈ O ₂	124.138	< B17	244	1	134.7	
4-Methoxyphenol	150-76-5	C ₇ H ₈ O ₂	124.138	57	243	0.485	134.7	
4-Chloroguaiacol	16766-30-6	C ₇ H ₇ ClO ₂	158.582	liquid		1	155.6	
5-Chloroguaiacol	3753-23-5	C ₇ H ₇ ClO ₂	158.582	34-35		0.807	155.6	
4,5-Dichloroguaiacol	2460-49-3	C ₇ H ₆ Cl ₂ O ₂	193.028	69-79		0.331	176.5	8.52
4,6-Dichloroguaiacol	2460-49-3	C ₇ H ₆ Cl ₂ O ₂	193.028	63-64		0.419	176.5	
3,4,5-Trichloroguaiacol	57057-83-7	C ₇ H ₃ Cl ₃ O ₂	227.473	85-86		0.255	197.4	7.56
4,5,6-Trichloroguaiacol	2668-24-8	C ₇ H ₃ Cl ₃ O ₂	227.473	112-115		0.137	197.4	7.2
Tetrachloroguaiacol	2539-17-5	C ₇ H ₄ Cl ₄ O ₂	261.918	121-122		0.113	218.3	6.26
Vanillin	121-33-5	C ₈ H ₈ O ₃	152.148	81.5	285	0.279	156.9	7.42
5-Chlorovanillin	19463-48-0	C ₈ H ₇ ClO ₃	185.593	165		0.0423	177.8	6.80
6-Chlorovanillin	18268-69-4	C ₈ H ₇ ClO ₃	185.593	171-172		0.0365	177.8	6.11

(Continued)

TABLE 14.2.1 (Continued)

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V_M cm ³ /mol		pK _a
							MW/ ρ at 20°C	Le Bas	
5,6-Dichlorovanillin	18113-22-9	C ₈ H ₆ Cl ₂ O ₃	221.038	198-199		0.0198		198.7	5.28
Syringol (2,6-Dimethoxyphenol)	91-10-1	C ₈ H ₁₀ O ₃	154.163	56.5	261	0.491		166.0	
3-Chlorosyringol	18113-22-9	C ₈ H ₉ ClO ₃	188.608	35-36		0.789		186.9	9.09
3,5-Dichlorosyringol	78782-46-4	C ₈ H ₈ Cl ₂ O ₃	223.054	105-106		0.162		207.8	7.27
Trichlorosyringol	2539-26-6	C ₈ H ₇ Cl ₃ O ₃	257.499	122-123		0.111		228.7	7.73
2-Chlorosyringaldehyde	76341-69-0	C ₉ H ₉ ClO ₄	216.619	196-197		0.0208		209.1	6.80
2,6-Dichlorosyringaldehyde	76330-06-8	C ₉ H ₈ Cl ₂ O ₄	251.064	195.6		0.0212		230.0	

* Assuming $\Delta S_{fus} = 56$ J/mol K.

TABLE 14.2.2

Summary of selected physical-chemical properties of phenolic compounds at 25°C

Compound	Selected properties					log K _{OW}	Henry's law constant H/(Pa·m ³ /mol) calculated P/C
	Vapor pressure		Solubility				
	P _S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		
Alkylphenols and other substituted phenols:							
Phenol	47	67.66	88360	938.9	1345	1.46	0.0500
<i>o</i> -Cresol (2-Methylphenol)		41	26000	240.4	237.32	1.98	0.1489
<i>m</i> -Cresol (3-Methylphenol)		16	22000	203.4	203.4	1.98	0.0786
<i>p</i> -Cresol (4-Methylphenol)		13	20000	184.9	230.6	1.96	0.0564
2,3-Dimethylphenol		8.05	6000	49.11	143.6		0.0560
2,4-Dimethylphenol		13.02	8795	71.99	71.99	2.35	0.1808
2,5-Dimethylphenol		10.68	3176	26.00	80.00		0.1335
2,6-Dimethylphenol		32.82	6230	51.00	81.60	2.36	0.4022
3,4-Dimethylphenol		2.241	5100	41.75	103.3	2.23	0.0217
3,5-Dimethylphenol		3.76	5500	45.02	107.2	2.35	0.0351
2,3,5-Trimethylphenol		2.43	800	5.874	28.24		0.0860
2,4,5-Trimethylphenol		7.73				2.67	
2,4,6-Trimethylphenol		19.58	1200	8.81	26.07	2.73	0.7511
3,4,5-Trimethylphenol		2.144	1540	11.31	73.91		0.0290
3-Methyl-5-ethylphenol		1.18	2314	16.99			
<i>o</i> -Ethylphenol		20.4	14042	114.9	114.9	2.47	0.1775
<i>m</i> -Ethylphenol		6.7				2.5	
<i>p</i> -Ethylphenol		5	7980	65.32	102.7	2.5	0.0487
2-Propylphenol		11.2				2.93	
4-Propylphenol		7.3	1728	12.69	12.69	3.2	0.5753
2-Isopropylphenol		12.45	4423	32.48	32.48	2.88	0.3834
4-Isopropylphenol			3263	23.96	55.59		
4-Butylphenol			617	4.107	4.107	3.65	
2- <i>sec</i> -Butylphenol		5				2.8	
2- <i>tert</i> -Butylphenol						2.7	
3- <i>tert</i> -Butylphenol			2070	13.78	20.38	2.6	
4- <i>sec</i> -Butylphenol		4	960	6.391	14.59	2.1	0.2741
4- <i>tert</i> -Butylphenol		1.24	580	3.861	20.11	3.04	0.0617
2-Methyl-5- <i>tert</i> -butylphenol		3.688	410	2.496			
2,6-Di- <i>sec</i> -butylphenol						4.4	

(Continued)

TABLE 14.2.2 (Continued)

Compound	Selected properties					log K _{OW}	Henry's law constant H/(Pa·m ³ /mol) calculated P/C
	Vapor pressure		Solubility				
	P _S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		
3,5-Di- <i>tert</i> -butylphenol			14	0.0678	0.2816		
2,6-Di- <i>tert</i> -butyl-4-methylphenol		0.0338				4.17	
3-Pentylphenol						3.13	
4-Hexylphenol			391	2.193	2.568	3.6	
2-Heptylphenol						4.45	
4-Heptylphenol						4.15	
4-Octylphenol		0.071	12.6	0.0611	0.0917	4.12	0.7743
4- <i>tert</i> -Octylphenol						3.7	
2-Nonylphenol						5.76	
3-Nonylphenol						5.61	
4-Nonylphenol		0.1	5.43	0.0246	0.0362	4.48	2.764
1-Naphthol		0.5	438	3.038	14.75	2.84	0.0339
2-Naphthol		0.4	740	5.133	45.42	2.7	8.81×10 ^{B3}
2-Phenylphenol		30	700	4.113	8.568	3.09	3.501
4-Phenylphenol		8.7	9.8	0.0576	1.391	3.2	6.256
2-Allylphenol						2.64	
Chlorophenols:							
2-Chlorophenol	132	132	24650	191.7	191.7	2.17	0.6884
3-Chlorophenol	35	41.57	22000	171.1	203.2	2.5	0.2045
4-Chlorophenol	20	29.90	27000	210.0	313.9	2.4	0.0952
2,3-Dichlorophenol			8215	50.40	106.3	3.15	
2,4-Dichlorophenol	12	18.87	4500	27.61	43.41	3.2	0.4347
2,5-Dichlorophenol						3.2	
2,6-Dichlorophenol	12	32.09	2625	16.10	43.06	2.86	0.7451
3,4-Dichlorophenol			9256	56.79	149.8	3.37	
3,5-Dichlorophenol			7394	45.36	119.7	3.2	
2,3,4-Trichlorophenol	1	3.74	500	2.532	9.484	3.8	0.3949
2,3,5-Trichlorophenol	1	2.31	500	2.532	5.848	3.69	0.3949
2,3,6-Trichlorophenol			450	2.279	4.808	3.8	
2,4,5-Trichlorophenol	2.5	6.76	948	4.801	12.98	3.72	0.5207
2,4,6-Trichlorophenol	1.25	3.44	434	2.198	5.941	3.69	0.5687
3,4,5-Trichlorophenol						4.3	

(Continued)

2,3,4,5-Tetrachlorophenol	0.1	0.79	166	0.7158	5.637	4.8	0.1397
2,3,4,6-Tetrachlorophenol	0.28	0.78	183	0.7892	2.180	4.45	0.3548
2,3,5,6-Tetrachlorophenol	0.1	0.78	100	0.4312	3.292	4.9	0.2319
Pentachlorophenol	4.15×10 ^{B3}	0.12	14	0.0526	1.524	5.05	0.0789
Nitrophenols:							
2-Nitrophenol		20	1080	7.764	12.15	1.8	1.646
3-Nitrophenol			11550	83.03	421.5	2	
4-Nitrophenol			13500	97.05	718.9	1.91	
2,4-Dinitrophenol			335	1.820	13.78	1.67	
2,4,6-Trinitrophenol (Picric acid)			13750	60.02	540.7	1.33	
4,6-Dinitro- <i>o</i> -cresol			222	1.120	4.500	2.12	
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:							
Catechol (1,2-Dihydroxybenzene)		1.34	45000	408.7	2462	0.88	5.44×10 ^{B4}
Resorcinol (1,3-Dihydroxybenzene)	0.0118	0.079	110000	999.0	6705	0.80	1.18×10 ^{B5}
Hydroquinone (1,4-Dihydroxybenzene)	2.55×10 ^{B3}	0.071	70000	635.7	17758	0.59	4.01×10 ^{B6}
2-Methoxyphenol (Guaiacol)	20.825	24.4	24800	199.8	233.9	1.33	0.1042
3-Methoxyphenol			67800	546.2	546.2	1.58	
4-Methoxyphenol			19500	157.1	323.9	1.34	
4-Chloroguaiacol			5370	33.86	33.86	2.15	
5-Chloroguaiacol			3960	24.97	30.94		
4,5-Dichloroguaiacol	0.570	1.72	575	2.98	9.000	3.26	0.1913
4,6-Dichloroguaiacol			708	3.668	8.754	2.86	
3,4,5-Trichloroguaiacol	0.163	0.64	310	1.363	5.344	3.77	0.1996
4,5,6-Trichloroguaiacol	0.032	0.23	54	0.2374	1.733	3.74	0.1348
Tetrachloroguaiacol	0.016	0.14	26	0.0993	0.8785	4.45	0.1612

TABLE 14.2.3

Suggested half-life classes for phenolic compounds in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Alkylphenols and other substituted phenols:				
Phenol	2	3	4	5
<i>o</i> -Cresol	1	2	3	4
<i>p</i> -Cresol	1	2	3	4
2,4-Dimethylphenol	2	3	4	5
Chlorophenols:				
2,4-Dichlorophenol	3	3	5	6
2,4,5-Trichlorophenol	4	4	6	7
2,4,6-Trichlorophenol	4	4	6	7
2,3,4,6-Tetrachlorophenol	5	5	6	7
Pentachlorophenol	5	5	6	7
Nitrophenols:				
2-Nitrophenol	3	3	5	6
4-Nitrophenol	3	3	5	6
2,4-Dinitrophenol	4	4	6	7
2,4,6-Trinitrophenol				
4,6-Dinitro- <i>o</i> -cresol	4	4	6	7
Dihydroxybenzenes, methoxyphenols and chloroguaiacols:				
Catechol	2	3	4	5
2-Methoxyphenol (Guaiacol)	2	3	4	5
Tetrachloroguaiacol	4	4	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

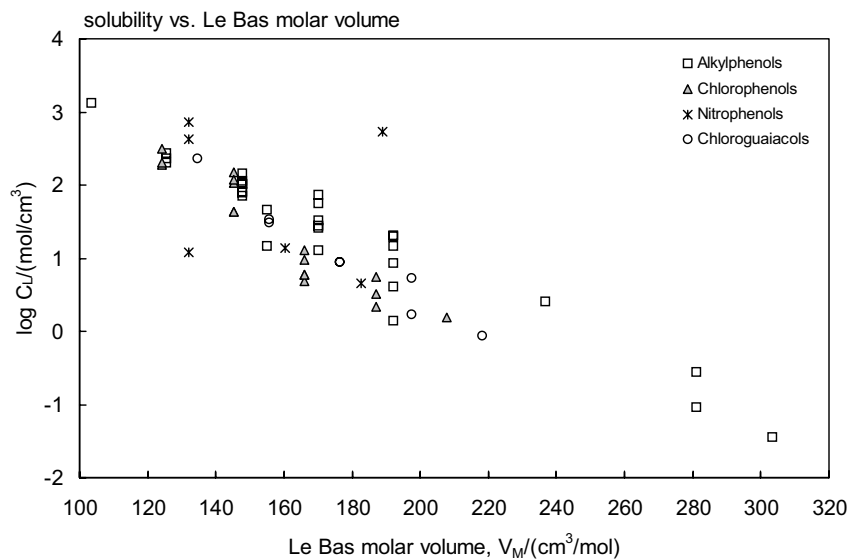


FIGURE 14.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.

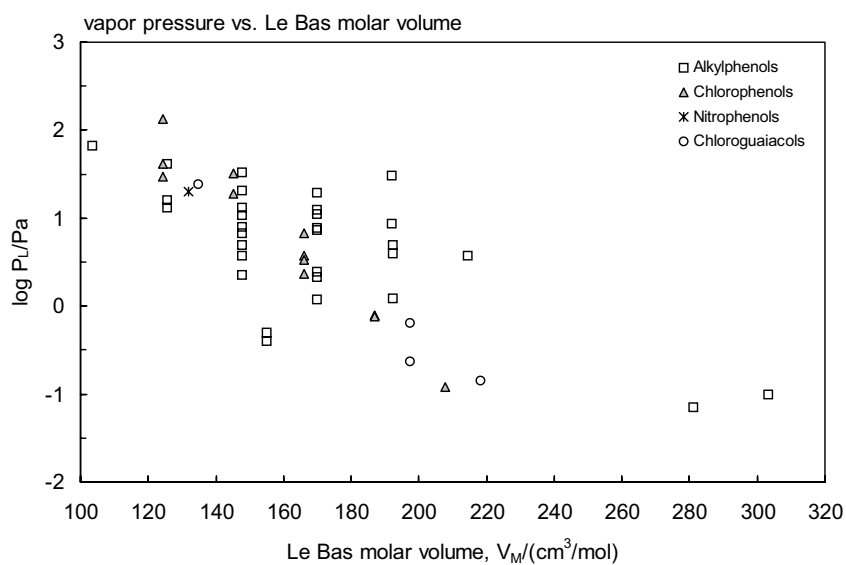


FIGURE 14.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for phenolic compounds.

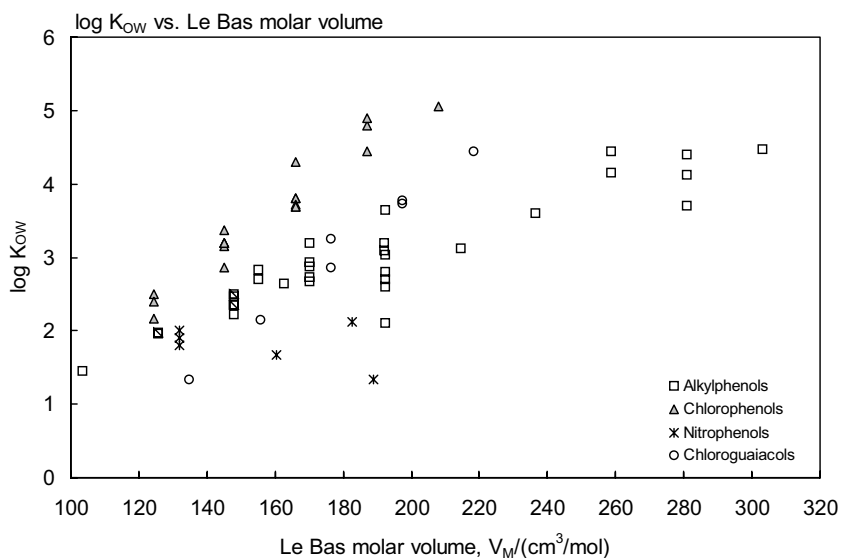


FIGURE 14.2.3 Octanol-water partition coefficient versus Le Bas molar volume for phenolic compounds.

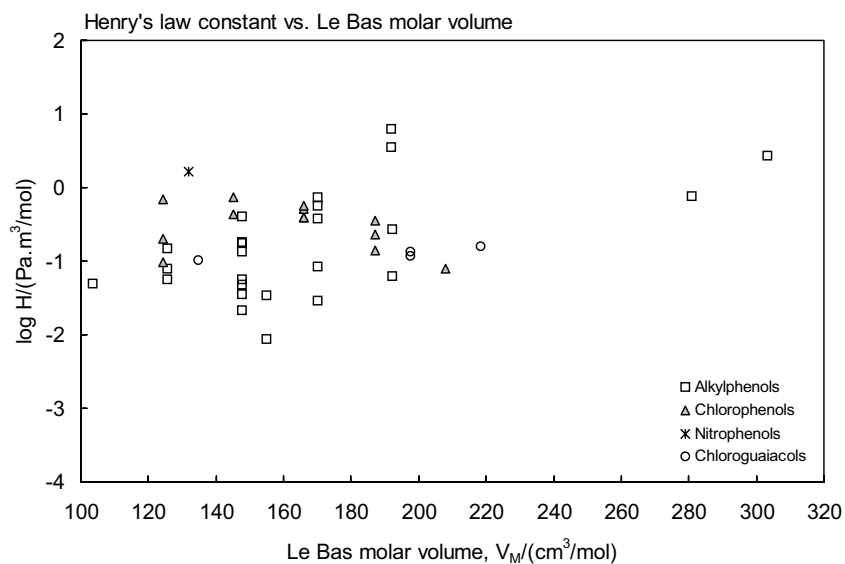


FIGURE 14.2.4 Henry's law constant versus Le Bas molar volume for phenolic compounds.

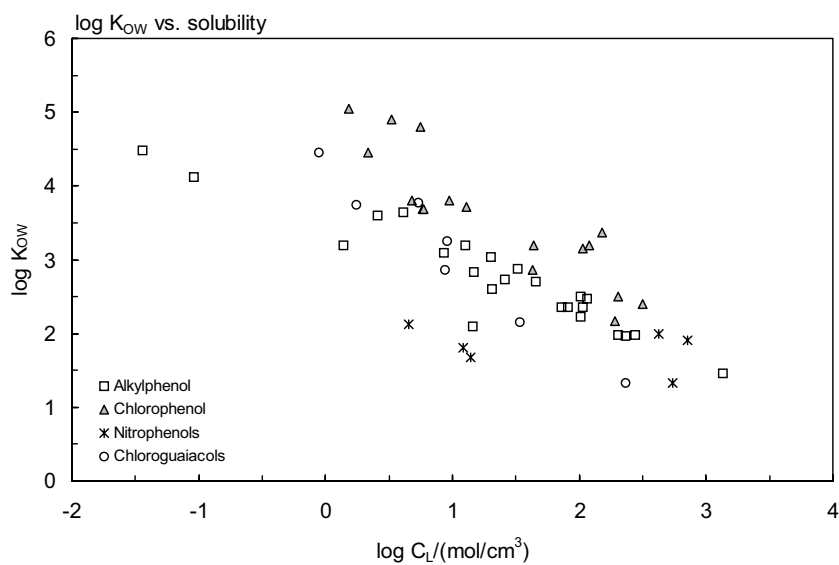


FIGURE 14.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for phenolic compounds.

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15 Esters

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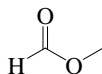
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15.1 LIST OF CHEMICALS AND DATA COMPILATIONS

15.1.1 ALIPHATIC ESTERS

15.1.1.1 Methyl formate



Common Name: Methyl formate

Synonym: formic acid methyl ester, methyl methanoate

Chemical Name: methyl formate

CAS Registry No: 107-31-3

Molecular Formula: $C_2H_4O_2$, $HCOOCH_3$

Molecular Weight: 60.052

Melting Point ($^{\circ}C$):

-99.0 (Weast 1982–83; Dean 1985; Lide 2003)

Boiling Point ($^{\circ}C$):

31.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9742 (Weast 1982–83)

0.9742, 0.9664 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

62.8 (exptl. at normal bp, Lee et al. 1972)

61.6 ($20^{\circ}C$, calculated-density)

62.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

30.59; 29.72 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

7.75 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

230000 (USEPA 1975; quoted, Howard 1993)

304000 ($20^{\circ}C$, Verschueren 1983)

230000 (Dean 1985; Riddick et al. 1986)

23800 (solubility data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

83260* (isoteniscope method, measured range 21 – $31.7^{\circ}C$, Nelson 1928)

$\log(P/mmHg) = 7.2202 - 1320.8/(T/K)$; temp range 21 – $31.7^{\circ}C$, Nelson 1928)

53329* ($16^{\circ}C$, summary of literature data, temp range -74.2 to $213^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 7027.8/(T/K)] + 7.852144$; temp range -74.2 to $213^{\circ}C$ (Antoine eq., Weast 1972–73)

63980, 93310 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

80840 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 2.11093 - 1.573/(-17.263 + t/^{\circ}C)$, temp range: 21 – $31.7^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

83440 (calculated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 3.207 - 3.02/(-11.9 + t/^{\circ}C)$, temp range: 21 – $32^{\circ}C$ (Antoine eq., Dean 1985, 1992)

78060 (selected lit., Riddick et al. 1986)

$\log(P/kPa) = 6.29529 - 1125.2/(174.2 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

78600 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.225693 - 1088.955/(-46.675 + T/\text{K})$; temp range 279–305 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.39684 - 1196.323/(-32.629 + T/\text{K})$; temp range 305–443 K (Antoine eq.-II, Stephenson & Malanowski 1987)

78070 (Daubert & Danner 1989)

$\log (P/\text{mmHg}) = 28.9576 - 2.3582 \times 10^3/(T/\text{K}) - 7.4848 \cdot \log(T/\text{K}) + 7.4384 \times 10^{-10} \cdot (T/\text{K}) + 2.7013 \times 10^{-6} \cdot (T/\text{K})^2$,
temp range 174–487 K (vapor pressure eq., Yaws 1994)

114881 (35°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

22.61 (exptl., Hine & Mookerjee 1975)

20.15, 17.96 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)

15.64 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

26.02 (calculated-P/C, Hoff et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

−0.010 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

−0.264 (estimated, Howard 1993)

0.03 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

1.75 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

−0.222 (estimated-S, Lyman et al. 1990)

Sorption Partition Coefficient, $\log K_{OC}$:

0.699 (soil, estimated-S, Lyman et al. 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant, $t_{1/2} \sim 5.3$ h from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1990; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius equation see reference:

$k_{OH} = (2.27 \pm 0.34) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 240–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a, quoted, Atkinson 1989)

$k_{OH}(\text{calc}) = 0.43 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: aqueous base-catalyzed hydrolysis $k = 36.6 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C corresponds to $t_{1/2} = 21.9$ d, 2.19 d, 9.1 h and 0.91 h at respective pHs of 6, 7, 8, and 9 (Mabey & Mill 1978; quoted, Howard 1993)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 74$ d, based on experimental reaction rate constant for the vapor-phase reaction with photochemically produced hydroxyl radical in the atmosphere at 23°C (Atkinson 1989; quoted, Howard 1993).

TABLE 15.1.1.1.1
Reported vapor pressures of methyl formate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
Nelson 1928	Stull 1947		
isoteniscope	summary of literature data		
t/°C	P/Pa	t/°C	P/Pa
21.0	80101	−74.2	133.3
25.0	83260	−57.0	666.6
26.6	86286	−48.6	1333
26.8	87286	−39.2	2666
27.1	88392	−28.7	5333
28.3	90406	−21.9	7999
28.9	94845	−12.9	13332
30.1	96378	0.80	26664
31.4	101431	16.0	53329
31.7	102351	32.0	101325
bp/°C	31.6	mp/°C	−99.8
eq. 1	P/mmHg		
A	7.2203		
B	1329.8		

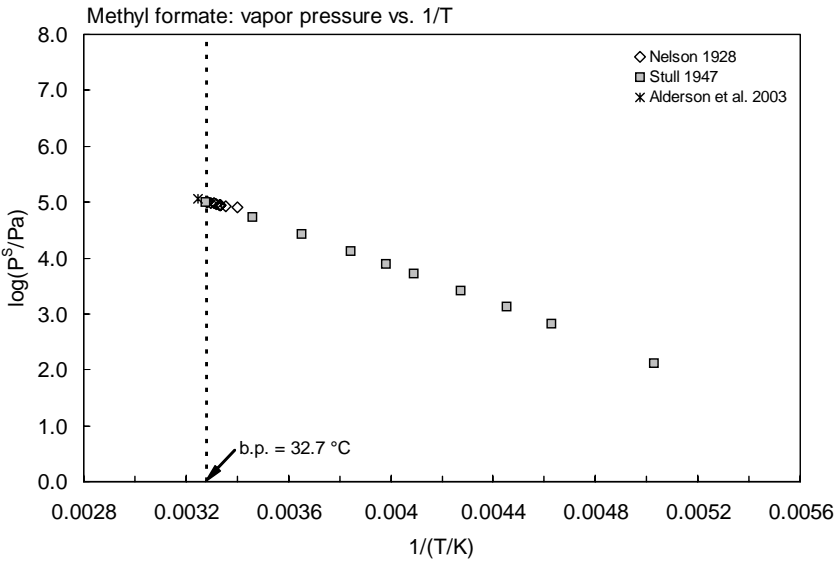
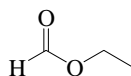


FIGURE 15.1.1.1.1 Logarithm of vapor pressure versus reciprocal temperature for methyl formate.

15.1.1.2 Ethyl formate



Common Name: Ethyl formate

Synonym: ethyl methanoate, formic acid ethyl ester

Chemical Name: ethyl formate

CAS Registry No: 109-94-4

Molecular Formula: $C_3H_6O_2$, $HCOOCH_2CH_3$

Molecular Weight: 74.079

Melting Point ($^{\circ}C$):

-79.6 (Lide 2003)

Boiling Point ($^{\circ}C$):

54.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9168 (Weast 1982-83)

0.9220, 0.9153 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

80.8 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

86.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

31.64; 29.94 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.205 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

88250 (Seidell 1941)

93260 (estimated, McGowan 1954)

52440 (Deno & Berkheimer 1960)

118000 (Verschueren 1983; Riddick et al. 1986)

117000 (Dean 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

34530* ($25.4^{\circ}C$, isoteniscope method, measured range 25.4 – $55.4^{\circ}C$, Nelson 1928)

$\log(P/mmHg) = 7.8457 - 1621.2/(T/K)$; temp range 25.4 – $55.4^{\circ}C$ (Nelson 1928)

33050* (interpolated-regression of tabulated data, temp range -60.5 to $54.3^{\circ}C$, Stull 1947)

30844* ($23.715^{\circ}C$, temp range 3.893 – $53.56^{\circ}C$, Mertl & Polak 1964 - ref. see Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 7511.7/(T/K)] + 7.842747$; temp range -60.5 to $225^{\circ}C$ (Antoine eq., Weast 1972-73)

25590, 39990 ($20^{\circ}C$, $30^{\circ}C$, Verschueren 1983)

30840, 32610 ($23.7^{\circ}C$, quoted exptl., interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.13263 - 1123.305/(218.177 + t/^{\circ}C)$; temp range 3.89 – $53.56^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

32540 (interpolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.0090 - 1123.94/(218.2 + t/^{\circ}C)$; temp range 4 – $54^{\circ}C$ (Antoine eq., Dean 1985, 1992)

32370 (selected, Riddick et al. 1986)

33070 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.1384 - 1151.08/[-48.94 + (T/K)]$; temp range: 213 – 336 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.4206 - 1326.4/[-26.867 + (T/K)]$; temp range: 327 – 498 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 29.9404 - 2.5263 \times 10^3/(T/K) - 7.809 \cdot \log(T/K) - 1.0111 \times 10^{-9} \cdot (T/K) + 2.7447 \times 10^{-6} \cdot (T/K)^2;$$

temp range 194–508 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

28.46	(exptl., Hine & Mookerjee 1975)
27.18, 25.96	(calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
17.55	(calculated-MCI χ , Nirmalakhandan & Speece 1988)
702.0	(calculated, Hoff et al. 1993)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

−0.38	(calculated, Iwasa et al. 1965)
0.23	(calculated, Hansch et al. 1968)
0.33	(Leo et al. 1971)
0.55	(calculated-intrinsic molar volume V_I and solvatochromic parameters, Leahy 1986)
0.26	(calculated-CLOGP, Müller & Klein 1992)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.19	(head-space GC, Abraham et al. 2001)
------	--------------------------------------

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (10.2 \pm 1.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a; quoted, Atkinson 1989)

$k_{\text{OH}} = 10.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988a)

$k_{\text{OH}}(\text{calc}) = 1.17 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 15.1.1.2.1

Reported vapor pressures of ethyl formate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Nelson 1928		Stull 1947		Mertl & Polak 1964	
isoteniscope		summary of literature data		ref in Boublik et al. 1984	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
25.4	34530	−60.5	133.3	3.893	11870
28.9	40103	−42.2	666.6	5.883	13155

(Continued)

TABLE 15.1.1.2.1 (Continued)

Nelson 1928		Stull 1947		Mertl & Polak 1964	
isoteniscope		summary of literature data		ref in Boublik et al. 1984	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
33.6	48263	-33.0	1333	8.963	15369
35.5	51982	-22.7	2666	12.395	18244
38.2	58555	-11.5	5333	16.185	21869
40.1	61608	-4.30	7999	19.290	25242
42.9	70914	5.40	13332	23.715	30844
44.2	72304	20.0	26664	28.260	37517
47.8	82193	40.0	53329	32.775	45345
50.9	91886	53.4	101325	38.220	56435
52.2	96139			43.630	69674
53.4	100392	mp/°C	-79	49.453	86066
54.2	102978			53.560	99805
55.4	109138				
bp/°C				eq. in Boublik et al. 1984	
53.8				eq. 2	P/kPa
				A	6.13263
eq. 1	P/mmHg			B	1123.305
A	7.8457			C	218.177
B	1621.6			bp/°C	54.013

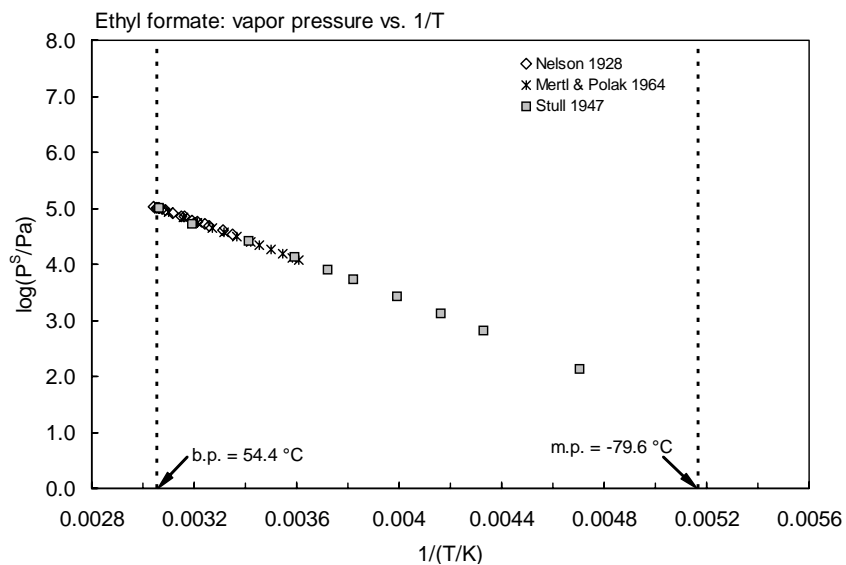
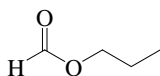


FIGURE 15.1.1.2.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl formate.

15.1.1.3 Propyl formate



Common Name: Propyl formate

Synonym: formic acid propyl ester, methanoic acid *n*-propyl ester, propyl methanoate

Chemical Name: *n*-propyl formate, propyl formate

CAS Registry No: 110-74-7

Molecular Formula: $C_4H_8O_2$, $HCOOCH_2CH_2CH_3$

Molecular Weight: 88.10 6

Melting Point ($^{\circ}C$):

−92.9 (Stull 1947; Weast 1982–83; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

80.9 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9058 (Weast 1982–83)

0.9006 (Dean 1985)

0.9055, 0.8996 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

97.3 ($20^{\circ}C$, calculated-density)

110.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

37.49; 33.60 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

28445 (Seidell 1941)

27230 (Deno & Berkheimer 1960)

27300 (Hansch et al. 1968; quoted, Hine & Mookerjee 1975; Müller & Klein 1992)

20500 (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

11759* ($26.2^{\circ}C$, isotenoscope method, measured range 26.2 – $82.3^{\circ}C$, Nelson 1928)

$\log(P/mmHg) = 7.9925 - 1806.5/(T/K)$; temp range 26.2 – $82.3^{\circ}C$ (Nelson 1928)

10620* (interpolated-regression of tabulated data, temp range -43 to $81.3^{\circ}C$ Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 8208.1/(T/K)] + 7.891833$; temp range -43 to $245^{\circ}C$ (Antoine eq., Weast 1972–73)

11010 (calculated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 5.98912 - 1135.489/(204.518 + t/^{\circ}C)$; temp range: 26.2 – $82.3^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

10710 (extrapolated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 6.848 - 1127/(203 + t/^{\circ}C)$; temp range: 26 – $82^{\circ}C$ (Antoine eq., Dean 1985, 1992)

11030 (quoted lit. average, Riddick et al. 1986)

$\log(P/kPa) = 5.97008 - 1132.3/(204.8 + t/^{\circ}C)$, temp range not specified (Antoine eq., Riddick et al. 1986)

10810 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.73268 - 1560.69/(-24.287 + T/K)$; temp range: 230 – 335 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.2378 - 1301.3/(-46.767 + T/K)$; temp range: 354 – 518 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log(P/\text{mmHg}) = 28.6983 - 2.6926 \times 10^3/(T/K) - 7.2435 \cdot \log(T/K) - 8.7226 \times 10^{-11} \cdot (T/K) + 1.9456 \times 10^{-6} \cdot (T/K)^2;$$

temp range 180–538 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 37.52 (exptl., Hine & Mookerjee 1975)
 38.39, 38.39 (calculated-group contribution, calculated-bond contribution, Hine & Mookerjee 1975)
 22.61 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 0.73 (calculated, Hansch et al. 1968)
 0.83 (shake flask, unpublished result, Leo et al. 1971; Hansch & Leo 1979)
 0.83 (recommended, Sangster 1989; 1993)
 0.83 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 2.66 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k_{\text{OH}} = (2.38 \pm 2.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988; quoted, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 1.87 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

TABLE 15.1.1.3.1

Reported vapor pressures of propyl formate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$	(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)		
<i>n</i> -propyl formate		isopropyl formate	
Nelson 1928		Stull 1947	
isoteniscope method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
26.2	11759	−43.0	133.3
30.8	14545	−22.7	666.6
35.2	17932	−12.6	1333
40.5	22718	−1.70	2666
Nelson 1928		Stull 1947	
isoteniscope method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
25.1	18198	−52.0	133.3
29.8	22585	−32.7	666.6
35.0	28958	−22.7	1333
41.2	37530	−12.1	2666

TABLE 15.1.1.3.1 (Continued)

n-propyl formate				isopropyl formate			
Nelson 1928		Stull 1947		Nelson 1928		Stull 1947	
isoteniscope method		summary of literature data		isoteniscope method		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
46.2	28864	10.8	5333	48.0	49062	0.20	5333
52.0	33717	18.8	7999	48.2	49609	7.50	7999
58.4	46516	29.5	13332	53.708	61101	17.8	13332
63.7	56235	45.3	26664	57.80	70661	33.6	26664
63.9	57422	62.6	53329	63.90	87726	50.5	53329
70.5	72034	81.3	101325	68.60	102405	68.3	101325
71.0	73967			70.30	108377		
73.5	79993	mp/°C	−92.5	77.788	113830	mp/°C	-
75.1	86513			72.100	116430		
78.9	96525						
80.5	101245			bp/°C	68.4		
82.3	106498			eq. 1	P/mmHg		
				A	7.8909		
				B	1710.5		
bp/°C	80.4						
eq. 1	P/mmHg						
A	7.99255						
B	1806.5						

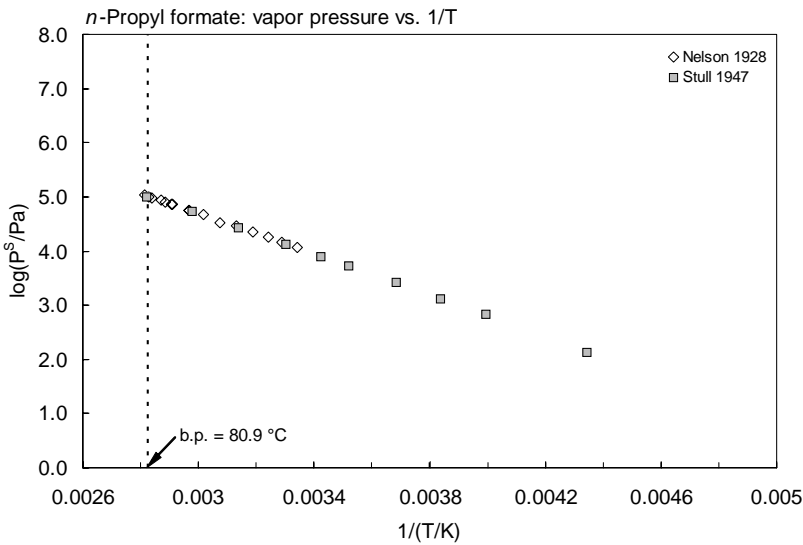


FIGURE 15.1.1.3.1 Logarithm of vapor pressure versus reciprocal temperature for n-propyl formate.

15.1.1.4 Methyl acetate



Common Name: Methyl acetate

Synonym: acetic acid methyl ester, ethanoic acid methyl ester, methyl ethanoate

Chemical Name: methyl acetate

CAS Registry No: 79-20-9

Molecular Formula: $C_3H_6O_2$, CH_3COOCH_3

Molecular Weight: 74.079

Melting Point ($^{\circ}C$):

-98.25 (Lide 2003)

Boiling Point ($^{\circ}C$):

56.89 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9330 (Weast 1982-83)

0.9342 (Dean 1985)

0.9342, 0.9279 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

79.3 ($20^{\circ}C$, calculated-density)

84.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

22.50 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

32.30, 30.33 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

243730 ($20^{\circ}C$, shake flask-turbidity, Fühner 1924)

294920 (estimated, McGowan 1954)

243500 ($20^{\circ}C$, Stephen & Stephen 1963)

240000, 319000 ($20^{\circ}C$, Verschueren 1983)

240000 (Dean 1985)

245000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

27980* (interpolated-regression of tabulated data, -52 to $57.8^{\circ}C$, Stull 1947)

25242* ($22.060^{\circ}C$, temp range 1.758 – $55.840^{\circ}C$, Mertl & Polak 1964; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 7732.8/(T/K)] + 7.938782$; temp range -57.2 to $225^{\circ}C$ (Antoine eq., Weast 1972-73)

28830* (ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.24410 - 1183.700/(T/K) - 50.736$; temp range 259.6 – $351.3 K$ (Antoine eq., ebulliometry, Ambrose et al. 1981)

31330 (Verschueren 1983)

28830 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.25449 - 1189.608/(223.115 + t/^{\circ}C)$; temp range -13.58 to $78.12^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.19357 - 1159.358/(219.913 + t/^{\circ}C)$; temp range 1.76 – $55.84^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

28200 (calculated-Antoine eq., Dean 1985)

$\log(P/mmHg) = 7.0652 - 1157.63/(219.73 + t/^{\circ}C)$; temp range: 1 – $56^{\circ}C$ (Antoine eq., Dean 1985, 1992)

28828 (lit. average, Riddick et al. 1986)

$\log (P/\text{kPa}) = 6.24410 - 1183.70/(222.414 + t/^{\circ}\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 28830, 28840 (interpolated-Antoine eq. I and II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.190152 - 1157.622/(-53.426 + T/\text{K})$; temp range 274–331 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 6.18771 - 1156.219/(-53.589 + T/\text{K})$; temp range: 274–331 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log (P/\text{mmHg}) = 33.7235 - 2.7204 \times 10^3/(T/\text{K}) - 9.1182 \cdot \log(T/\text{K}) - 9.4316 \times 10^{-11} \cdot (T/\text{K}) + 3.3102 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 175–507 K (vapor pressure eq., Yaws 1994)
 53808 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

9.190 (volatility-partial pressure, Butler & Ramchandani 1935)
 11.65 (volatility-partial pressure-GC, Buttery et al. 1969)
 8.795 (exptl., Hine & Mookerjee 1975)
 11.59, 9.210 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
 13.06 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, $\Delta H = 39.2 \text{ kJ/mol}$, Kieckbusch & King 1979)
 9.210, 25.96 (quoted, calculated-MCI χ , Nirmalakhandan & Speece 1988)
 9.80 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 4.590 - 2048/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

0.18 (shake flask-CR, Collander 1951; quoted, Hansch & Leo 1979; Hansch & Leo 1985)
 0.23 (calculated, Hansch et al. 1968)
 0.70 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
 0.18 (recommended, Sangster 1989, 1993)
 0.18 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

2.31 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

-0.224 (calculated-S, Lyman et al. 1982)
 -0.092 (calculated- K_{OW} , Lyman et al. 1982)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

0.681 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1993)
 1.474 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on calculated Henry's law constant, $t_{1/2} \sim 9.1 \text{ h}$ from a model river of 1 m deep flowing at 1 m/s with wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = (1.1 \pm 0.03) \times 10^{10} \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or $(1.7 \pm 0.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 292 K using relative rate technique for *n*-butane (Campbell & Parkinson 1978)

$k_{\text{OH}}(\text{exptl}) = (1.3 - 3.41) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güesten et al. 1984; Atkinson 1987; Wallington et al. 1988a,b; quoted, Howard 1993)

$k_{\text{OH}}(\text{calc}) = 1.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 1.7 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (3.41 \pm 0.29) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (absolute rate, flash photolysis-resonance fluorescence, Wallington 1988a)

$k_{\text{OH}} = 3.41 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 2.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}}(\text{calc}) = 6.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.182 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

atmospheric $t_{1/2} = 47\text{--}94 \text{ d}$, based on exptl. rate constants for the vapor-phase reaction with photochemically produced hydroxyl radical in air (Atkinson et al. 1979; Güesten et al. 1984; Atkinson 1987; Wallington et al. 1988; quoted, Howard 1993).

Surface water:

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.1.4.1

Reported vapor pressures of methyl acetate at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)		
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)		
log P = A – B/(C + T/K)		(3)					
log P = A – B/(T/K) – C·log (T/K)		(4)					
Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		ref. in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
–57.2	133.3	1.758	9202	–13.581	3785	57.559	103841
–38.6	666.6	4.058	10415	–10.401	4597	61.773	119919
–29.3	1333	6.568	11870	–7.621	5426	65.575	136076
–19.1	2666	8.563	13155	–4.400	6450	70.114	157575
–7.90	5333	11.635	15369	–1.427	7733	74.442	180470
–0.50	7999	15.145	18244	1.819	9241	78.128	202007
9.40	13332	18.975	21869	4.978	10938	25.0	28828
24.0	26664	22.060	25242	8.278	12977		
40.0	53329	26.520	30844	11.635	15386	bp/K	330.018
57.8	101325	31.060	37517	14.886	18029		
		35.590	45345	19.151	22079	Antoine eq.	
mp/°C	–98.7	41.090	56435	22.787	26098	eq. 3	P/kPa
		46.500	69474	26.948	31418	A	6.24410
		52.310	86066	31.023	37456	B	1184.700
		55.840	97512	35.319	44810	C	–50.735

TABLE 15.1.1.4.1 (Continued)

Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		ref. in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
				40.047	54206		
				44.148	63603	data also fitted to: Chebyshev equation and Chebyshev polynomial coefficients given in ref.	
				48.507	74964		
				53.215	89039		
				56.821	101164		

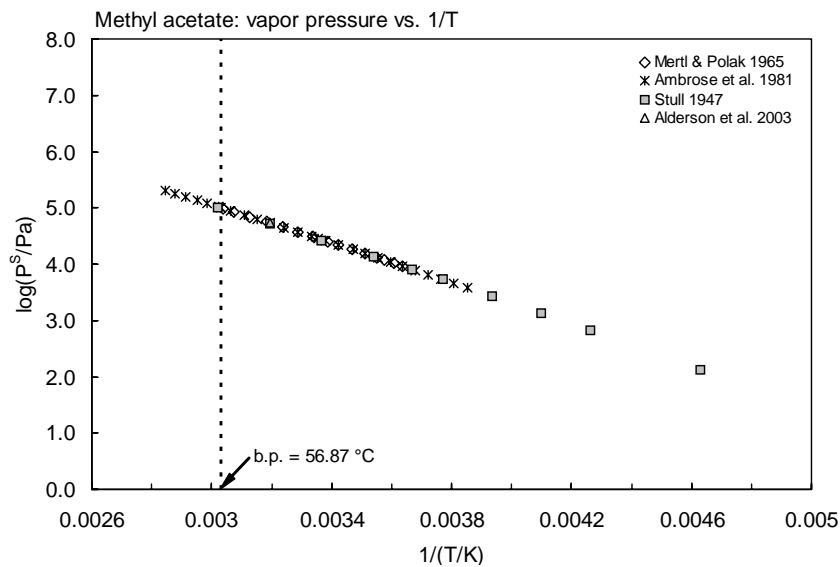
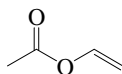


FIGURE 15.1.1.4.1 Logarithm of vapor pressure versus reciprocal temperature for methyl acetate.

15.1.1.5 Vinyl acetate



Common Name: Vinyl acetate

Synonym: ethanoic acid ester, ethenyl acetate, ethenyl ethanoate

Chemical Name: ethenyl acetate, vinyl acetate

CAS Registry No: 108-05-4

Molecular Formula: $C_4H_6O_2$, $CH_3COOCH=CH_2$

Molecular Weight: 86.090

Melting Point ($^{\circ}C$):

−93.2 (Weast 1982–83; Lide 2003)

Boiling Point ($^{\circ}C$):

72.8 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9317 (Weast 1982–83)

Molar Volume (cm^3/mol):

92.2 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

101.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

37.2, 34.35 ($25^{\circ}C$, bp. Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

19722 (Deno & Berkheimer 1960)

25000 (Verschuereen 1983)

20000 (Dean 1985)

20000 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

14454* (interpolated-regression of tabulated data, temp range -48 to $72.5^{\circ}C$, Stull 1947)

21.83* ($21.83^{\circ}C$, measured range 21.8 – $72.04^{\circ}C$, Capkova & Fried 1964 - ref see Boublik et al. 1984)

84406* ($67^{\circ}C$, vapor-liquid equilibrium data, measured range 67 – $82^{\circ}C$, Swamy & Van Winkle 1965)

15300 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 7.17023 - 1766.918/(269.951 + t/^{\circ}C)$; temp range: 67 – $82^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.3363 - 1296.847/(226.731 + t/^{\circ}C)$; temp range: 21.83 – $72.04^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

15300 (interpolated-Antoine eq., Dean 1985, 1992)

$\log(P/mmHg) = 7.2101 - 1296.13/(226.66 + t/^{\circ}C)$; temp range: 22 – $72^{\circ}C$ (Antoine eq., Dean 1985, 1992)

14100 (quoted lit. average, Riddick et al. 1986)

$\log(P/kPa) = 7.216 - 1798.4/(T/K)$; temp range: not specified (Antoine eq., Riddick et al. 1986)

15340, 15305 (interpolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.3799 - 1320.2716/(-43.96 + T/K)$; temp range: 293 – 346 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.34264 - 1300.315/(-46.041 + T/K)$; temp range 294 – 346 K (Antoine eq.-II, Stephenson & Malanowski 1987)

11320 ($20^{\circ}C$, quoted, Howard 1989)

$$\log (P/\text{mmHg}) = 12.722 - 2.177 \times 10^3/(T/K) - 91.458 \cdot \log (T/K) - 4.5688 \times 10^{-3} \cdot (T/K) + 2.9673 \times 10^{-6} \cdot (T/K)^2;$$

temp range 180–524 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

48.74 (calculated-P/C, Howard 1989)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.60 (shake flask, Fujisawa & Masuhara 1980)
0.21 (calculated-HPLC-RT, Fujisawa & Masuhara 1981)
0.73 (recommended, Sangster 1989, 1993)
0.73 (recommended, Hansch et al. 1995)

Bioconcentration Factor, $\log \text{BCF}$:

0.32–0.37 (estimated- K_{ow} , Howard 1989)

Sorption Partition Coefficient, $\log K_{oc}$:

1.28–1.77 (estimated- K_{ow} , Howard 1989)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 4.4$ h from a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s, and $t_{1/2} = 2.2$ d from an environmental pond (Howard 1989).

Photolysis:

Oxidation: $t_{1/2} = 13$ and 8 d for reactions with OH radical and singlet oxygen in sunlit natural water (Howard 1989).

Hydrolysis: overall rate constant $k_h = 1.10 \times 10^{-6} \text{ s}^{-1}$ with $t_{1/2} = 7.3$ d at 25°C and pH 7 (Mabey & Mill 1978)
degradation $t_{1/2} = 7.3$ d at 25°C and pH 7, the hydrolysis rate will increase as the pH increases (Howard 1989).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: estimated $t_{1/2} = 12$ h with photochemically produced hydroxyl radical in an average atmosphere (Howard 1989).

Surface water: hydrolysis degradation $t_{1/2} = 7.3$ days at 25°C and pH 7; $t_{1/2} = 13$ and 8 d for reactions with hydroxyl radical and singlet oxygen, respectively, in natural water (Howard 1989).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.1.5.1
Reported vapor pressures of vinyl acetate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}C)$		(2)	$\ln P = A - B/(C + t/^{\circ}C)$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Capkova & Fried 1963		Swamy & Van Winkle 1965	
summary of literature data		in Boublik et al. 1984		V-L equil. data	
t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa	t/ $^{\circ}C$	P/Pa
-48.0	133.3	21.83	13159	67.0	84406
-28.0	666.6	25.12	15372	69.0	90646
-18.0	1333	28.8	18252	70.0	92899
-7.0	2666	32.85	21891	72.0	100711
5.30	5333	36.13	25264	74.0	107924
13.0	7999	40.82	30864	76.0	115550
23.3	13332	45.64	37543	78.0	123643
38.4	26664	50.37	45356	80.0	132189
55.5	53329	56.12	56448	82.0	131215
72.5	101325	61.83	69487		
		67.92	86046		
mp/ $^{\circ}C$	-73	72.04	99958		
		eq. 2	P/kPa		
		A	6.33630		
		B	1296.847		
		C	226.731		
		bp/ $^{\circ}C$	71.731		

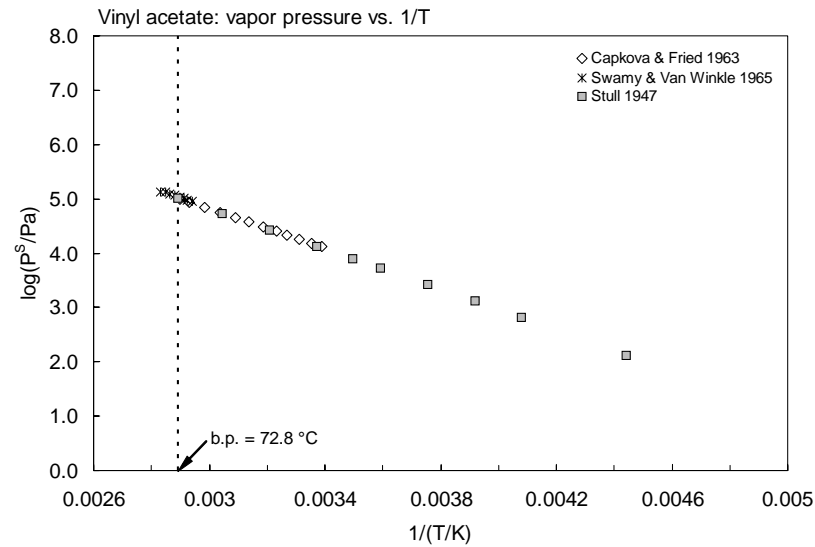
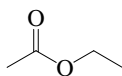


FIGURE 15.1.1.5.1 Logarithm of vapor pressure versus reciprocal temperature for vinyl acetate.

15.1.1.6 Ethyl acetate



Common Name: Ethyl acetate

Synonym: acetic acid ethyl ester, acetic ether, ethanoic acid ester, ethyl ethanoate

Chemical Name: *n*-ethyl acetate, ethyl acetate

CAS Registry No: 141-78-6

Molecular Formula: $C_4H_8O_2$, $CH_3COOCH_2CH_3$

Molecular Weight: 88.106

Melting Point ($^{\circ}C$):

−83.8 (Lide 2003)

Boiling Point ($^{\circ}C$):

77.11 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9003 (Weast 1982–83)

0.9006, 0.8946 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

106.0 (exptl. at normal bp, Lee et al. 1972)

97.8 ($20^{\circ}C$, calculated-density)

108.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

22.83 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

35.62, 31.97 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

10.50 (Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

64408 ($20^{\circ}C$, shake flask-turbidity, Fühner 1924)

85300 ($20^{\circ}C$, synthetic method, Jones 1929)

78720 (shake flask-centrifuge, Booth & Everson 1948)

80100* (turbidimetric method, measured range 20 – $40^{\circ}C$, Altshuller & Everson 1953)

80400* (average, Altshuller & Everson 1953)

79780 (shake flask-interferometry, Donahue & Bartell 1952)

69990 (estimated, McGowan 1954)

82220 (Deno & Berkheimer 1960)

80350 (shake flask-UV, Hansch et al. 1968)

63960 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)

82500, 74000 ($20^{\circ}C$, $35^{\circ}C$, literature average, Verschueren 1983)

80000 (shake flask-HPLC, Banerjee 1984)

97000 (Dean 1985)

95000 (shake flask-radiometric method, Lo et al. 1986)

80800 (lit. average, Riddick et al. 1986)

77900* ($20.2^{\circ}C$, shake flask-GC/TC, measured range 0 – $70^{\circ}C$, Stephenson & Stuart 1986)

73700 (solubility data compilation, Yaws et al. 1990)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

13330*, 11860 ($27.0^{\circ}C$, interpolated-regression of tabulated data, temp range -43.4 to $78.1^{\circ}C$, Stull 1947)

$\log(P/mmHg) = 7.30588 - 1357.7/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

- 13155* (25.86°C, temp range 15.58–75.830°C, Mertl & Polak 1964; quoted, Boublik et al. 1984)
 $\log(P/\text{mmHg}) = [-0.2185 \times 8301.1/(T/K)] + 8.001170$; temp range –43.4 to 235°C (Antoine eq., Weast 1972–73)
- 12600* (ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)
 $\log(P/\text{kPa}) = 6.18799 - 1224.673/(T/K) - 57.438$; temp range: 271–372.865 K (Antoine eq., ebulliometry, Ambrose et al. 1981)
- 9704 (20°C, Verschueren 1983)
- 11220 (calculated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.1171 - 1245.172/(217.984 + t/^{\circ}\text{C})$, temp range 15.58–75.83°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.20229 - 1232.542/(216.587 + t/^{\circ}\text{C})$, temp range –2.08 to 99.71°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
- 12620 (calculated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.10179 - 1244.95/(217.88 + t/^{\circ}\text{C})$ temp range 15–76°C (Antoine eq., Dean 1985, 1992)
- 12600 (lit. average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.18799 - 1224.673/(215.712 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
- 12620 (interpolated-Antoine eq.-I and III, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.227229 - 1245.239/(-55.239 + T/K)$; temp range: 288–351 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.38462 - 1369.41/(-37.675 + T/K)$; temp range: 350–508 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.22825 - 1245.68/(-55.193 + T/K)$; temp range: 288–351 K (Antoine eq.-III, Stephenson & Malanowski 1987)
- 3240, 5240 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 0.6955 - 2.2498 \times 10^3/(T/K) + 5.4643 \cdot \log(T/K) - 1.9451 \times 10^{-2} \cdot (T/K) + 1.2362 \times 10^{-5} \cdot (T/K)^2$;
temp range 190–623 K (vapor pressure eq., Yaws 1994)
- 25078 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 13.42 (partial pressure, Butler & Ramchandani 1935)
- 17.78 (28°C, concn. ratio-GC, Nelson & Hoff 1968)
- 13.62 (exptl., Hine & Mookerjee 1975)
- 15.64, 13.94 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
- 17.20 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, $\Delta H = 41.4 \text{ kJ/mol}$, Kieckbusch & King 1979)
- 13.62, 24.22 (quoted, calculated-MCI χ , Nirmalakhandan & Speece 1988)
- 41.72* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 $\ln(1/K_{AW}) = -7.28 + 3563/(T/K)$, temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)
- 13.62, 6.23 (quoted, calculated-molecular structure, Russell et al. 1992)
- 11.33 (calculated, Hoff et al. 1993)
- 13.51 (solid-phase microextraction SPME-GC, Bartelt 1997)
- 12.72 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 5.095 - 2163/(T/K)$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 0.66 (shake flask-chemical reaction CR, Collander 1951)
- 0.73 (shake flask-GC, Hansch & Anderson 1967; quoted, Leo et al. 1969, 1971; Hansch & Leo 1979)
- 0.73 (shake flask-UV, Hansch et al. 1968; Hansch & Leo 1979)
- 0.65, 0.66 (calculated- π substituent const.; calculated-fragment const., Rekker 1977)
- 0.70 (exptl., Valvani et al. 1981; quoted, Amidon & Williams 1982)
- 0.53 (calculated-activity coeff. γ , Wasik et al. 1981)
- 0.68 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
- 1.02 (calculated-activity coeff. γ from UNIFAC, Banerjee & Howard 1988)
- 0.73 (recommended, Sangster 1989, 1993)
- 0.73 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

2.70 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

4.13 (alga *Chlorella fusca*, wet wt. basis, Geyer et al. 1984)
 0.70 (alga *Chlorella fusca*, calculated- K_{OW} , Geyer et al. 1984)
 1.48 (golden ide, Freitag et al. 1985)
 4.13 (algae, Freitag et al. 1985)
 3.52 (activated sludge, Freitag et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

0.361 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 10.1$ h was estimated for a model river of 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1990).

Photolysis: rate constant $k = 6.8 \times 10^{-4} \text{ h}^{-1}$ to $2.21 \times 10^{-3} \text{ h}^{-1}$ with H_2O_2 under photolysis at 25°C in F-113 solution and with HO^- in the gas (Dilling et al. 1988).

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures and/or Arrhenius equation see reference:

photooxidation $t_{1/2} = 2.75\text{--}110$ yr in water, based on measured rate constant for the reaction with hydroxyl radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991)

photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{OH} = (1.16 \pm 0.13) \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 292 K using relative rate technique for *n*-butane (Campbell & Parkinson 1978)

$k_{OH}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.82 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{OH}(\text{calc}) = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{OH}(\text{obs.}) = 1.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{OH}^* = (15.1 \pm 1.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K, measured range 296–440 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a; quoted Atkinson 1989)

$k_{OH} = 1.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 6.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{OH} = 1.6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{OH}(\text{calc}) = 1.94 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.110 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988);

overall rate constant $k_h = 1.10 \times 10^{-8} \text{ s}^{-1}$ with $t_{1/2} = 2.0$ yr at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 2.02$ yr, based on measured rate constants for acid and base catalyzed and neutral hydrolysis at pH 7 and 20°C (Mabey & Mill 1978; quoted, Howard 1990; Howard et al. 1991; Kollig 1993)

$t_{1/2} = 9.5 \times 10^7$ d at pH 2, $t_{1/2} = 740$ d at pH 7 and $t_{1/2} = 97000$ d at pH 12 in natural waters at $20\text{--}25^\circ\text{C}$ (Capel & Larson 1995)

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated aqueous aerobic biodegradation screening test data (Heukelekian & Rand 1955; Price et al. 1974; selected, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 4$ d in natural waters (Capel & Larson 1995)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.75\text{--}110$ yr, based on measured rate constant for the reaction with OH radical in water (Dorfman & Adams 1973; selected, Howard et al. 1991);

$t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976);

photodecomposition $t_{1/2} = 14.6$ h under simulated atmospheric conditions, with NO (Dilling et al. 1976)

photooxidation $t_{1/2} = 35.3\text{--}353$ h, based on measured rate constant for the reaction with OH radical in air (Atkinson 1985; selected, Howard et al. 1991);

calculated lifetimes of 6.9 d and 10 yr for reactions with OH radical, NO_3 radical, respectively (Atkinson 2000).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1$ d, $t_{1/2}(\text{anaerobic}) = 4$ d; hydrolysis $t_{1/2} = 9.5 \times 10^7$ d at pH 2, $t_{1/2} = 740$ d at pH 7 and $t_{1/2} = 97000$ d at pH 12 in natural waters at $20\text{--}25^\circ\text{C}$ (Capel & Larson 1995)

Groundwater: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 15.1.1.6.1

Reported aqueous solubilities and Henry's law constants of ethyl acetate at various temperatures

Aqueous solubility				Henry's law constant	
Altshuller & Everson 1953		Stephenson & Stuart 1986		Kolb et al. 1992	
synthetic method-turbidity		shake flask-GC/TC		equilibrium headspace-GC	
$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$	$t/^\circ\text{C}$	$H/(\text{Pa}\cdot\text{m}^3 \text{ mol}^{-1})$
20	83200	0	97100	40	41.72
25	80100	9.5	86200	60	94.53
30	77000	20.0	77900	70	130.9
35	73900	30.0	68100	80	167.8
40	70800	40.0	62800		
		50.0	62000	$\ln (1/K_{\text{AW}}) = A - B/(T/K)$	
eq.	$S/(\text{g}/100\text{g})$	59.9	60600	A	-7.28
$S = 9.552 - 0.0618 \cdot (t/^\circ\text{C})$		70.5	58800	B	-3563
summary of lit. average					
20	84200				
25	80400				
30	77000				
35	73900				
40	71200				

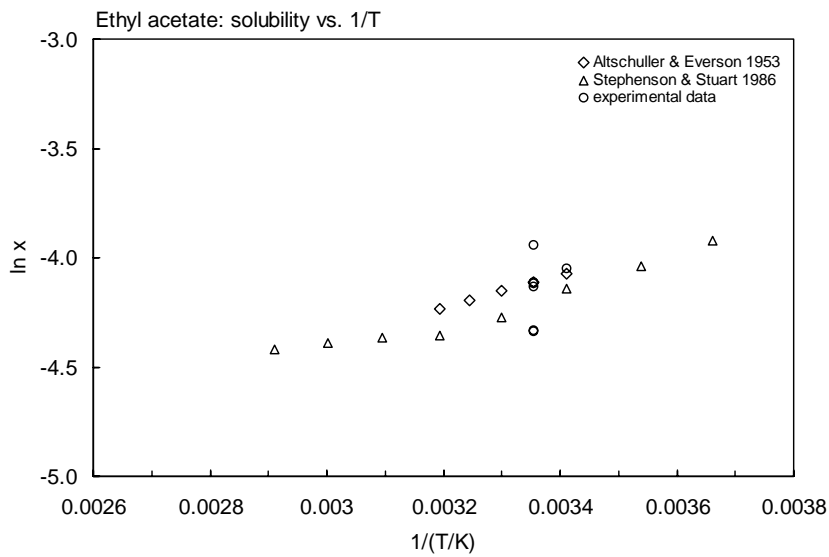


FIGURE 15.1.1.6.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for ethyl acetate.

TABLE 15.1.1.6.2
Reported vapor pressures of ethyl acetate at various temperatures and the coefficients for the vapor pressure equations

log P = A – B/(T/K)		(1)	ln P = A – B/(T/K)		(1a)				
log P = A – B/(C + t/°C)		(2)	ln P = A – B/(C + t/°C)		(2a)				
log P = A – B/(C + T/K)		(3)							
log P = A – B/(T/K) – C·log (T/K)		(4)							
Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981					
summary of literature data		in Boublik et al. 1984		comparative ebulliometry					
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa		
–43.4	133.3	15.58	7838	–2.07	2868	29.112	15339		
–23.5	666.6	18.58	9202	–0.096	3236	32.553	17990		
–13.5	1333	21.115	10415	2.398	3754	37.060	22031		
–3.0	2666	23.775	11870	5.737	4560	40.920	26056		
9.10	5333	25.86	13155	8.692	5385	45.333	31374		
16.6	7999	29.135	15369	12.098	6494	49.657	37046		
27.0	13332	32.830	18244	15.242	7683	54.214	44760		
42.0	26664	36.875	21869	18.681	9187	59.231	54168		
59.3	53329	40.175	25242	22.022	10878	63.588	63565		
77.1	101325	44.905	30844	25.532	12925	68.218	74938		
mp/°C	–82.4	49.715	37517	29.119	15336	73.224	89016		
		54.505	45345	32.599	17990	77.056	101144		
		60.320	56435	37.086	22033	77.053	103823		
		66.045	69474	40.929	26056	82.321	119902		
		72.190	86066	25.0	12600	86.359	136066		
		75.830	97272	bp/K	350.261	91.183	157571		
		eq. 2	P/kPa			95.786	180471		
						99.715	202018		
		A	6.22710	Antoine eq.					

(Continued)

TABLE 15.1.1.6.2 (Continued)

Stull 1947		Mertl & Polak 1965		Ambrose et al. 1981			
summary of literature data		in Boublik et al. 1984		comparative ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
		B	1245.172	eq. 3	P/kPa	data also fitted to:	
		C	217.904	A	6.18799	Chebyshev equation and	
		bp	77.064	B	1224.673	Chebyshev polynomial	
				C	-57.438	coefficients given in ref.	
						bp/°C	77.115
						Bublik	P/kPa
						A	6.20229
						B	1232.542
						C	216.587

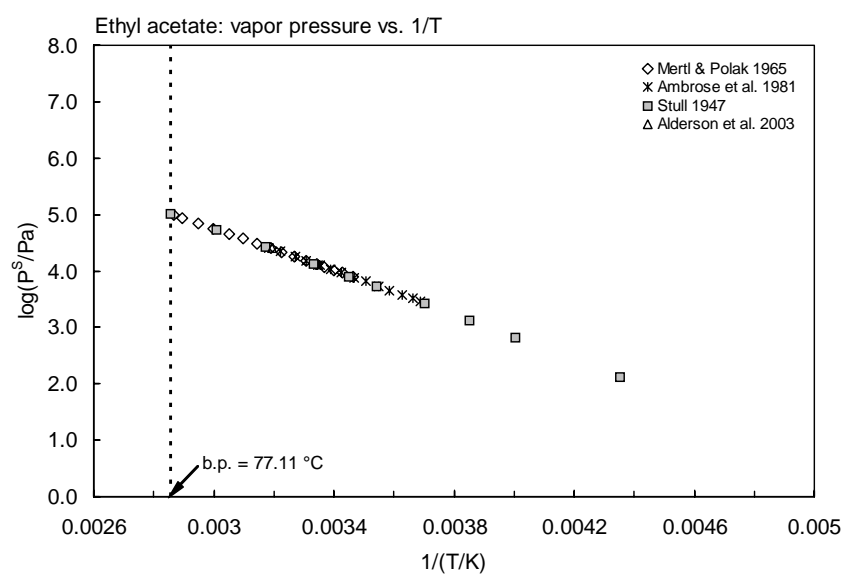
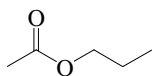


FIGURE 15.1.1.6.2 Logarithm of vapor pressure versus reciprocal temperature for ethyl acetate.

15.1.1.7 Propyl acetate



Common Name: Propyl acetate

Synonym: acetic acid propyl ester, propyl ethanoate, *n*-propyl acetate

Chemical Name: propyl acetate, *n*-propyl acetate

CAS Registry No: 109-60-4

Molecular Formula: $C_5H_{10}O_2$, $CH_3COOCH_2CH_2CH_3$

Molecular Weight: 102.132

Melting Point ($^{\circ}C$):

−93 (Lide 2003)

Boiling Point ($^{\circ}C$):

101.54 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8878 (Weast 1982–83)

0.8830 ($25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

115.0 ($20^{\circ}C$, calculated-density)

133.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

−7.18 (Perrin 1972)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

39.83, 33.86 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperature designated * are compiled at the end of this section):

18895 ($20^{\circ}C$, shake flask-turbidity, Fühner 1924)

18890 (Fühner 1924; quoted, Hansch et al. 1968)

20380 (estimated, McGowan 1954)

18160 (quoted, Deno & Berkheimer 1960)

18900 (Stephen & Stephen 1963; quoted, Howard 1993)

18895 (shake flask-UV, Hansch et al. 1968)

20430 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)

22450 ($20^{\circ}C$, literature average, Verschueren 1983)

23000 (Dean 1985)

23000 ($20^{\circ}C$, lit. average, Riddick et al. 1986)

22600*, 19800 ($20^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.2^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4152* (interpolated-regression of tabulated data, temp range -26.7 to $101.8^{\circ}C$ Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 8794.8/(T/K)] + 8.212268$; temp range -38.3 to $89^{\circ}C$ (Antoine eq., Weast 1972–73)

4478 (comparative ebulliometry, fitted to Antoine eq., Ambrose et al. 1981)

$\log(P/kPa) = 6.14362 - 1284.080/(T/K) - 64.364$; temp range 290.3 – 398.908 K (Antoine eq., ebulliometry, Ambrose et al. 1981)

4494 (interpolated-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 6.16547 - 1297.186/(210.301 + t/^{\circ}C)$; temp range 17.13 – $125.8^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.14152 - 1282.545/(208.628 + t/^{\circ}C)$; temp range 39.8 – $100.9^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

- 4486 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.01615 - 1282.28/(208.6 + t/^{\circ}\text{C})$, temp range: 39–101°C (Antoine eq., Dean 1985, 1992)
 4497 (quoted lit average, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.14362 - 1284.080/(208.786 + t/^{\circ}\text{C})$, temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 6.142106 - 1282.873/(-64.486 + T/\text{K})$; temp range 312–374 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.48937 - 1544.31/(-30.623 + T/\text{K})$; temp range 374–542 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.13951 - 1281.682/(-64.58 + T/\text{K})$; temp range 312–374 K (Antoine eq.-III, Stephenson & Malanowski 1987)
 $\log(P/\text{mmHg}) = 43.0548 - 3.4692 \times 10^3/(T/\text{K}) - 12.217 \cdot \log(T/\text{K}) + 2.4748 \times 10^{-10} \cdot (T/\text{K}) + 3.7508 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 178–549 K (vapor pressure eq., Yaws et al. 1994)
 9586 (40°C, vapor-liquid equilibrium VLE data, Alderson et al. 2003)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations):

- 20.150 (exptl., Hine & Mookerjee 1975)
 22.092, 20.62 (calculated-group contribution, bond contribution, Hine & Mookerjee 1975)
 22.09 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C, data presented in graph, $\Delta H = 43.2 \text{ kJ/mol}$, Kieckbusch & King 1979)
 30.50 (calculated-MCI χ , Nirmalakhandan & Speece 1988)
 82.91, 203.7, 290.5, 387.3 (40, 60, 70 80°C, equilibrium headspace-GC, Kolb et al. 1992)
 $\ln(1/K_{\text{AW}}) = -9.27 + 3971/(T/\text{K})$, temp range 40–80°C (equilibrium headspace-GC, Kolb et al. 1992)
 10.10 (calculated-molecular structure, Russell et al. 1992)
 16.13 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 5.519 - 2257/(T/\text{K})$, (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.23 (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)
 1.11 (calculated-activity coeff. γ , Wasik et al. 1981)
 1.24 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
 1.23 (Hansch & Leo 1985)
 1.24 (recommended, Sangster 1989, 1993)
 1.24 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 3.17 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.380, 0.708 (calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.288, 2.045 (soil, calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: based on Henry's law constant, $t_{1/2} \sim 6.5 \text{ h}$ from a model river of one meter deep flowing at 1 m/s with a wind velocity of 3 m/s (Lyman et al. 1982; quoted, Howard 1993).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

exptl. photooxidation rate constant of 2.4 to $4.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the vapor-phase reaction with the photochemically produced hydroxyl radicals in the atmosphere (Conkle et al. 1975; Atkinson et al. 1979; Ambrose et al. 1981; Atkinson 1985, 1987; Drossman et al. 1988; quoted, Howard 1993)

photooxidation half-life of 2.4–24 h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}} = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $305 \pm 2 \text{ K}$ using relative rate technique for 2-methylpropene (Winer et al. 1977; quoted, Atkinson 1985)

$k_{\text{OH}} = (1.7 \pm 0.2) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (Zetzsch 1982; quoted, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1985)

$k_{\text{OH}}(\text{calc}) = 2.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 2.51 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp. (SAR structure-activity relationship, Atkinson 1987)

$k_{\text{OH}} = (34.5 \pm 3.4) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988a)

$k_{\text{OH}} = 3.45 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{soln}) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for reaction with OH radical in aqueous solution (Wallington et al. 1988b)

$k_{\text{OH}} = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

$k_{\text{OH}}(\text{calc}) = 2.54 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (molecular orbital calculations, Klamt 1996)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.087 \text{ M}^{-1} \text{ s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radicals (Darnall et al. 1976);

$t_{1/2} = 3.39\text{--}6.69 \text{ d}$, based on exptl. rate constant for the vapor-phase reaction with the photochemically produced hydroxyl radical in the atmosphere (Conkle et al. 1975; Atkinson et al. 1979; Ambrose et al. 1981; Atkinson 1985, 1987; Drossman et al. 1988; quoted, Howard 1993).

TABLE 15.1.1.7.1
Reported aqueous solubilities of propyl acetate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

$t/^\circ\text{C}$	$\text{S/g}\cdot\text{m}^{-3}$
0	32100
9.5	27800
20.0	22600
30.0	19800
40.0	18700
50.0	17200
60.1	16400
70.5	17200
80.0	16600
90.2	13500

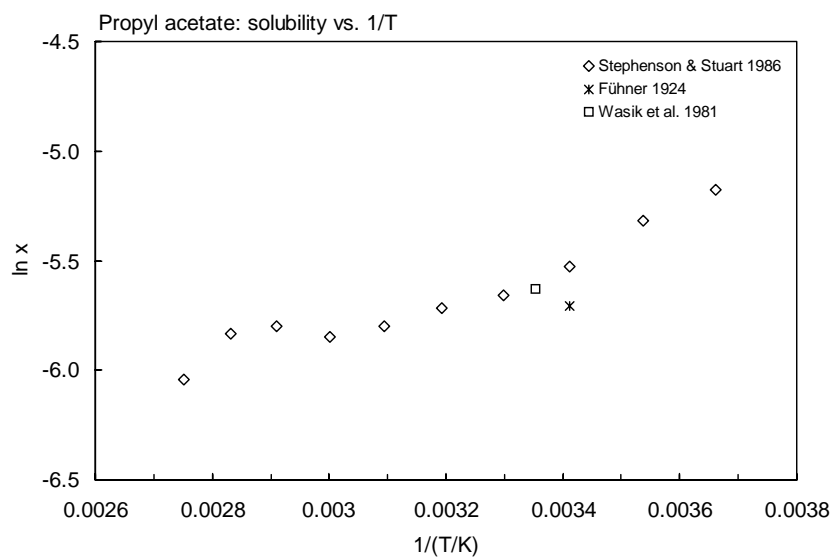


FIGURE 15.1.1.7.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for propyl acetate.

TABLE 15.1.1.7.2

Reported vapor pressures of propyl acetate at various temperatures

Stull 1947

summary of literature data

t/°C	P/Pa
-26.7	133.3
-5.40	666.6
5.0	1333
16.0	2666
28.8	5333
37.0	7999
47.8	13332
64.0	26664
82.0	53329
101.8	101325
mp/°C	-92.5

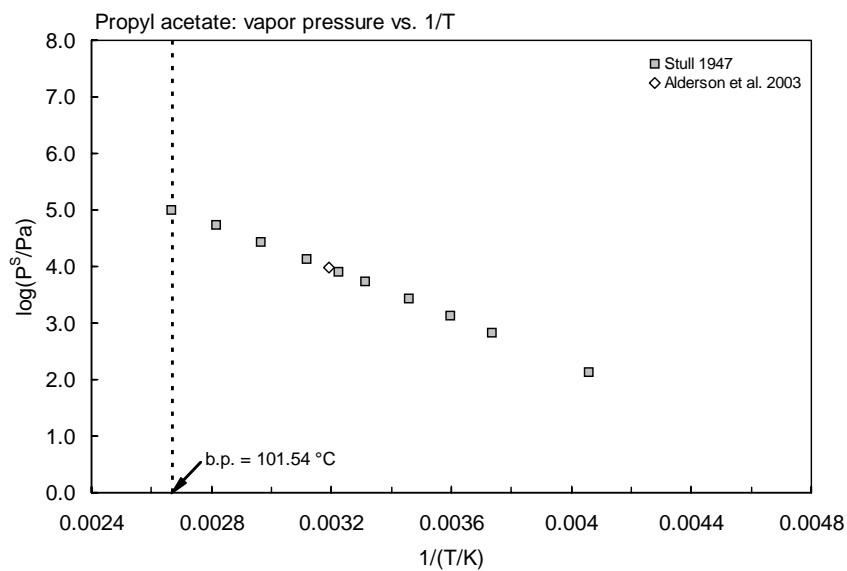
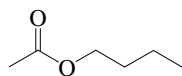


FIGURE 15.1.1.7.2 Logarithm of vapor pressure versus reciprocal temperature for propyl acetate.

15.1.1.8 Butyl acetate



Common Name: Butyl acetate

Synonym: acetic acid butyl ester, butyl ethanoate, *n*-butyl acetate, ethanoic acid butyl ester

Chemical Name: butyl acetate, *n*-butyl acetate

CAS Registry No: 123-86-4

Molecular Formula: $C_6H_{12}O_2$, $CH_3COOCH_2CH_2CH_2CH_3$

Molecular Weight: 116.158

Melting Point ($^{\circ}C$):

-78 (Lide 2003)

Boiling Point ($^{\circ}C$):

126.1 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8825 (Weast 1982-83)

0.8764 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

132.5 ($20^{\circ}C$, calculated-density)

155.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

23.28 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

43.64, 35.81 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

23550 (Seidell 1941)

23180 (estimated, McGowan 1954)

4955 (Deno & Berkheimer 1960)

23580 (shake flask-spectrophotometry, Hansch et al. 1968)

7040 ($20^{\circ}C$, quoted, Amidon et al. 1975)

6702 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)

3936 (Hine & Mookerjee 1975)

5000, 14000 (Verschuieren 1983)

4300 (Dean 1985)

8400 (shake flask-radiometric method, Lo et al. 1986)

6800 ($20^{\circ}C$, quoted lit. average, Riddick et al. 1986)

6400*, 5200 ($19.7^{\circ}C$, $30.3^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.5^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

$\log (P/mmHg) = 8.099 - 1964/(253 + t/^{\circ}C)$ (Davis 1941)

1560* ($24.5^{\circ}C$, measured range 24.5 – $94.1^{\circ}C$, Usanovich & Dembicij 1959)

9210* ($59.74^{\circ}C$, temp range 59.74 – $126.09^{\circ}C$, Kliment et al. 1964; quoted, Boublik et al. 1984)

3386* ($67.9^{\circ}C$, ebulliometry, measured range 67.9 – $124.0^{\circ}C$, Sheehan & Langer 1969)

1505 (Hoy 1970)

$\log (P/mmHg) = 6.9688 - 1326.7/(199.2 + t/^{\circ}C)$; temp range 67.0 – $130^{\circ}C$ (ebulliometry, Sheehan & Langer 1969)

$\log (P/mmHg) = [-0.2185 \times 9300.8/(T/K)] + 8.095046$; temp range -21.2 to $118^{\circ}C$ (Antoine eq., Weast 1972-73)

1440 (quoted, Hine & Mookerjee 1975)

- 1333 (20.0°C, Verschueren 1983)
 1530, 1138 (extrapolated-Antoine eq., interpolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 6.25496 - 1432.217/(210.936 + t/^\circ\text{C})$; temp range 59.74–126°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log(P/\text{kPa}) = 4.7514 - 669.809/(117.657 + t/^\circ\text{C})$; temp range 24.5–94.1°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 1529 (extrapolated-Antoine eq., Dean 1985)
 $\log(P/\text{mmHg}) = 7.12712 - 1430.418/(210.746 + t/^\circ\text{C})$; temp range 60–126°C (Antoine eq., Dean 1985, 1992)
 1664 (selected, Riddick et al. 1986)
 $\log(P/\text{kPa}) = 6.151445 - 1368.051/(203.9298 + t/^\circ\text{C})$; temp range not specified (Antoine eq., Riddick et al. 1986)
 $\log(P_L/\text{kPa}) = 6.176 - 1385.8/(-67.05 + T/\text{K})$; temp range 332–399 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.13505 - 1355.816/(-70.705 + T/\text{K})$; temp range: 341–399 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 2000, 635 (measured, calculated-solvatochromic parameters, Banerjee et al. 1990)
 $\log(P/\text{mmHg}) = 4.383 - 2.7134 \times 10^3/(T/\text{K}) + 3.9835 \cdot \log(T/\text{K}) - 1.6575 \times 10^{-2} \cdot (T/\text{K}) + 9.7246 \times 10^{-6} \cdot (T/\text{K})^2$; temp range 200–579 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 33.44 (exptl., Hine & Mookerjee 1975)
 30.50, 31.21 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)
 28.51 (vapor-liquid equilibrium, headspace-GC, measured range 25–40°C data presented in graph, $\Delta H = 47.6 \text{ kJ/mol}$, Kieckbusch & King 1979)
 38.39 (predicted-MCI χ , Nirmalakhandan & Speece 1988)
 82.91* (40°C, equilibrium headspace-GC, measured range 40–80°C, Kolb et al. 1992)
 20.2 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{\text{AW}} = 6.400 - 2486/(T/\text{K})$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 1.73 (calculated, Hansch et al. 1968; quoted, Leo et al. 1969)
 1.69 (calculated-activity coeff. γ , Wasik et al. 1981)
 1.82 (generator column-GC, Wasik et al. 1981, 1982; Tewari et al. 1982)
 1.78 (24°C, shake flask-GC, Catz & Friend 1989)
 1.82 (recommended, Sangster 1989, 1993)
 1.78 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$ at 25°C:

- 3.65 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log \text{BCF}$:

- 0.602, 1.146 (calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 1.531, 2.367 (soil, calculated-S, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1990)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: using Henry's law constant, $t_{1/2} \sim 6.1 \text{ h}$ was estimated for a model river 1 m deep flowing at 1 m/s with a wind velocity of 3 m/s and an estimated $t_{1/2} \sim 7.4 \text{ d}$ for a 10 m deep similar model river (Lyman et al. 1982; quoted, Howard 1990).

Photolysis:

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

photooxidation $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976)

$k_{\text{OH}}(\text{calc}) = 4.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_{\text{OH}}(\text{obs.}) = 4.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at room temp.
(SAR structure-activity relationship, Atkinson 1987)

photooxidation $t_{1/2} = 6.0 \text{ d}$ in air was estimated for the vapor-phase reaction with an average atmospheric OH of $8 \times 10^5/\text{cm}^3$ (GEMS 1986; quoted, Howard 1990)

$k_{\text{OH}} = (41.5 \pm 3.0) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K (flash photolysis-resonance fluorescence, Wallington et al. 1988)

$k_{\text{OH}} = 4.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (recommended, Atkinson 1989)

Hydrolysis: alkaline hydrolysis rate constant $k = 0.087 \text{ M}^{-1}\cdot\text{s}^{-1}$ at 25°C in water (Salmi & Leimu 1947; quoted, Drossman et al. 1988);

$t_{1/2} = 3.1 \text{ yr}$, 114 d, 11.4 d at pH 7.0, 8.0, 9.0 were estimated, respectively, based on observed acid and base-catalyzed rate constants at 20°C (Mabey & Mill 1978; quoted, Howard 1990).

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: $t_{1/2} = 2.4\text{--}24 \text{ h}$ for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976);

$t_{1/2} = 6.0 \text{ d}$ was estimated for the vapor-phase reaction with an average atmospheric hydroxyl radical of $8 \times 10^5 \text{ per cm}^3$ (GEMS 1986; quoted, Howard 1990).

TABLE 15.1.1.8.1
Reported aqueous solubilities and Henry's law constants of
butyl acetate at various temperatures

Aqueous solubility		Henry's law constant	
Stephenson & Stuart 1986		Kolb et al. 1992	
shake flask-GC/TC		equilibrium headspace-GC	
t/°C	S/g·m ⁻³	t/°C	H/(Pa m ³ mol ⁻¹)
0	9600	40	82.91
9.1	7600	60	203.7
19.7	6400	70	290.5
30.3	520	80	387.3
39.6	500		
50.0	500	$\ln (1/K_{\text{AW}}) = A - B/(T/K)$	
60.2	500	A	-9.27
70.2	470	B	-3971
80.1	480		
90.5	480		

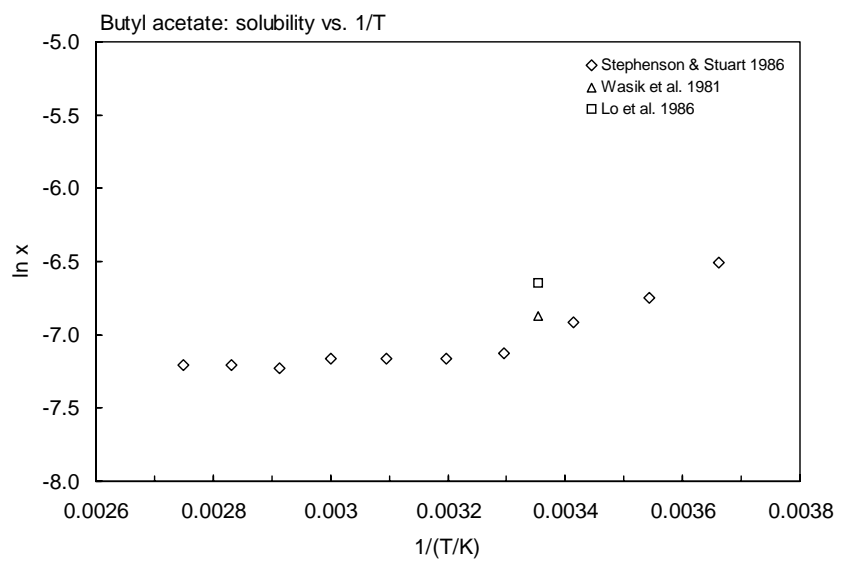


FIGURE 15.1.1.8.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for butyl acetate.

TABLE 15.1.1.8.2
Reported vapor pressures of butyl acetate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)		
$\log P = A - B/(C + t/^{\circ}C)$	(2)	$\ln P = A - B/(C + t/^{\circ}C)$	(2a)		
$\log P = A - B/(C + T/K)$	(3)				
$\log P = A - B/(T/K) - C \cdot \log (T/K)$	(4)				
Usanovich & Dembicij 1959	Kliment et al. 1964	Sheehan & Langer 1969			
in Boublik et al. 1984	in Boublik et al. 1984	ebulliometry			
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
24.5	1560	59.74	9210	67.9	13386
33.0	2533	62.35	10426	96.3	40183
43.0	4133	65.52	11876	100	45663
51.2	6199	67.96	13159	124.0	97325
57.7	8533	71.70	15372		
65.2	11999	75.88	18252	Antoine eq.	
71.1	15332	80.49	21891	eq. 2	P/mmHg
77.5	20132	84.21	25264	A	6.9688
83.7	25598	89.58	30864	B	1326.7
88.8	31064	95.06	37543	C	199.2
94.1	42130	100.53	45356		
		107.07	56448		
eq in Boublik et al. 1984		113.62	69487		
eq. 2	P/kPa	120.62	86053		
A	4.75140	126.09	101325		
B	669.609				
C	117.657	eq in Boublik et al. 1984			
bp/°C	60.892	eq. 2	P/kPa		
	at 10 mmHg	A	6.25496		
		B	1432.217		
		C	218.936		
		bp/°C	126.116		

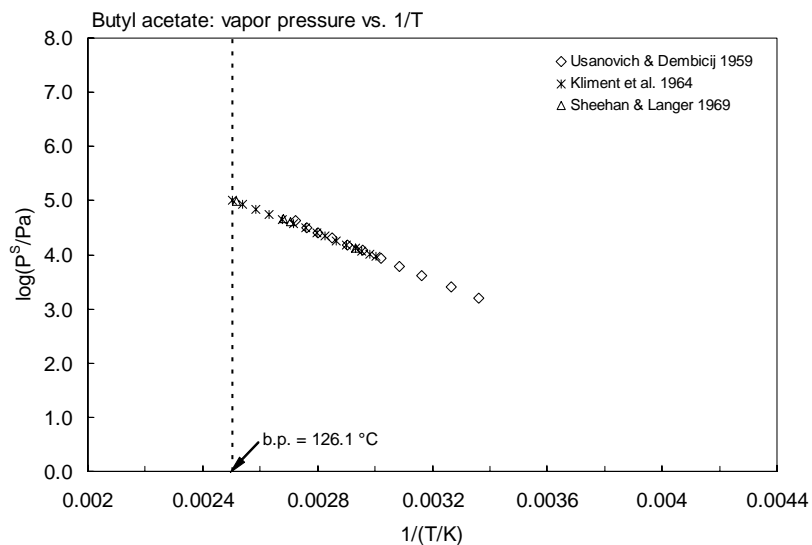
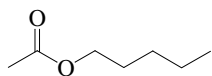


FIGURE 15.1.1.8.2 Logarithm of vapor pressure versus reciprocal temperature for butyl acetate.

15.1.1.9 Pentyl acetate



Common Name: Pentyl acetate

Synonym: acetic acid pentyl ester, amyl acetate, amylacetic ester, pentyl ethanoate, *n*-pentyl acetate, ethanoic acid pentyl ester

Chemical Name: *n*-amyl acetate, *n*-pentyl acetate

CAS Registry No: 628-63-7

Molecular Formula: $C_7H_{14}O_2$, $CH_3COOCH_2CH_2CH_2CH_2CH_3$

Molecular Weight: 130.185

Melting Point ($^{\circ}C$):

-70.8 (Weast 1982–83; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

149.2 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.8756 (Weast 1982–83)

0.8766, 0.8719 ($20^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

148.5 ($20^{\circ}C$, calculated-density)

177.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant:

24.25 (pK_s , Riddick et al. 1986)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.0 (at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1730 (shake flask-turbidimeter, McBain & Richards 1946)

1800 ($20^{\circ}C$, Verschueren 1983)

1700 (Dean 1985)

1700 ($20^{\circ}C$, Riddick et al. 1986)

2200*, 1600 ($19.7^{\circ}C$, $30.3^{\circ}C$, shake flask-GC/TC, measured range 0 – $80^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 8.078 - 2077/(253 + t/^{\circ}C)$ (Davis 1946)

547 (quoted, Hine & Mookerjee 1975)

546 (quoted, Abraham 1984)

1290 (selected lit., Riddick et al. 1986)

$\log(P/kPa) = 5.4315 - 1197/(200 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 7.356 - 2258.3/(T/K)$; temp range 329–423 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 7.8848 - 3.0696 \times 10^3/(T/K) + 2.7085 \cdot \log(T/K) - 1.5165 \times 10^{-2} \cdot (T/K) + 8.7135 \times 10^{-6} \cdot (T/K)^2$; temp range 202–598 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

39.29 (exptl., Hine & Mookerjee 1975)

42.10, 42.16 (calculated-group contribution, calculated-group contribution, Hine & Mookerjee 1975)

35.94 (vapor-liquid equilibrium, headspace-GC, measured range 25 – $40^{\circ}C$ data presented in graph, $\Delta H = 51.4$ kJ/mol, Kieckbusch & King 1979)

48.33 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

- 38.39 (calculated-molecular structure, Russell et al. 1992)
 24.86 (20°C, selected from literature experimentally measured data, Staudinger & Roberts 2001)
 $\log K_{AW} = 7.167 - 2685/(T/K)$ (van't Hoff eq. derived from literature data, Staudinger & Roberts 2001)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 1.70 (calculated, Iwasa et al. 1965)
 2.23 (Leo et al. 1969)
 2.42 (calculated- V_1 and solvatochromic parameters, Leahy 1986)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 4.12 (head-space GC, Abraham et al. 2001)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with OH radical in air, based on the rate of disappearance of hydrocarbon due to reaction with OH radical (Darnall et al. 1976).

Hydrolysis:

Biodegradation: biodegradation rates $k = 0.054\text{ d}^{-1}$ with $t_{1/2} = 13$ d in Lester river, $k = 0.069\text{ d}^{-1}$ with $t_{1/2} = 10$ d in Superior harbor waters and $k = 0.014\text{ d}^{-1}$ with $t_{1/2} = 50$ d in groundwater (Vaishnav & Babeu 1987).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.4\text{--}24$ h for the gas-phase reaction with hydroxyl radical in air, based on the rate of disappearance of hydrocarbon due to reaction with hydroxyl radical (Darnall et al. 1976).

Surface water: biodegradation $t_{1/2} = 13$ d in Lester river and $t_{1/2} = 10$ d in Superior harbor waters (Vaishnav & Babeu 1987).

Groundwater: biodegradation $t_{1/2} = 50$ d (Vaishnav & Babeu 1987).

Sediment:

Soil:

Biota:

TABLE 15.1.1.9.1
Reported aqueous solubilities of pentyl acetate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	2900
19.7	2200
30.6	1600
39.5	1600
50.0	1000
60.3	1000
70.2	1700
80.1	1700

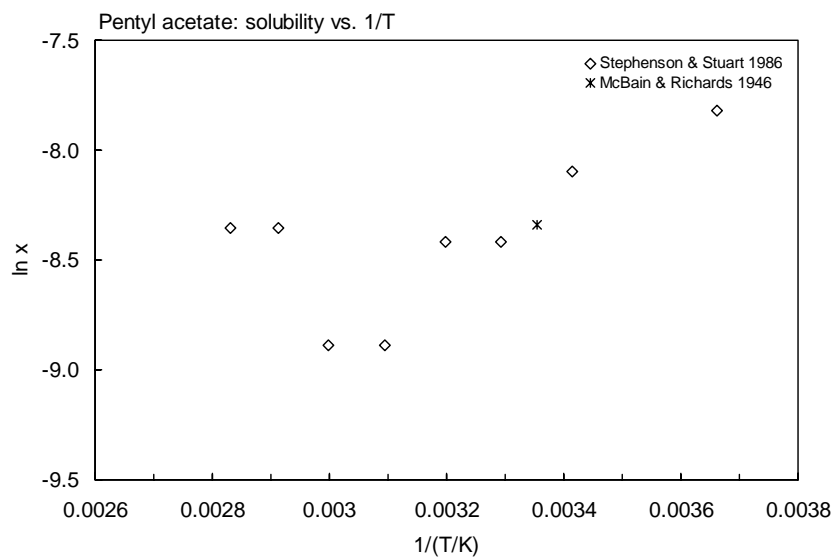
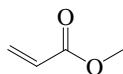


FIGURE 15.1.1.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for pentyl acetate.

15.1.1.10 Methyl acrylate



Common Name: Methyl acrylate

Synonym: acrylic acid methyl ester, methyl 2-propenoate

Chemical Name: methyl acrylate

CAS Registry No: 96-33-3

Molecular Formula: $C_4H_6O_2$, $CH_2=CHCOOCH_3$

Molecular Weight: 86.090

Melting Point ($^{\circ}C$):

-76.5 (Dean 1985)

Boiling Point ($^{\circ}C$):

80.7 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9535 (Weast 1982-83; Riddick et al. 1986)

0.9561 (Dean 1985)

Molar Volume (cm^3/mol):

90.3 ($20^{\circ}C$, calculated-density)

99.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

29.20, 33.1 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

60000 (Dean 1985)

49400 (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

11250 (interpolated-regression of tabulated data, temp range -43.7 to $80.2^{\circ}C$, Stull 1947)

13330 ($28.0^{\circ}C$, Stull 1947)

$\log(P/\text{mmHg}) = [-0.2185 \times 8598.0/(T/K)] + 8.226778$; temp range -43.7 to $80.2^{\circ}C$ (Antoine eq., Weast 1972-73)

9330, 14660 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

11000 (Riddick et al. 1986)

3120, 5400, 9090, 11000, 14500, 30000, 70700 (0, 10, 20, 25, 30, 50, $70^{\circ}C$, Riddick et al. 1986)

$\log(P_L/\text{kPa}) = 6.5561 - 1467.93/(-30.849 + T/K)$; temp range: 316-354 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/\text{mmHg}) = 47.0416 - 3.1218 \times 10^3/(T/K) - 14.86 \cdot \log(T/K) + 7.1646 \times 10^{-3} \cdot (T/K) + 3.4547 \times 10^{-6} \cdot (T/K)^2$; temp range 196-536 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

19.17 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.21 (Tute 1971; Laurence et al. 1972)

0.36 (HPLC-RT correlation, Fujisawa & Masuhara 1981)

0.80 (shake flask-GC, Tani & Hashimoto 1982)

0.80 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.7\text{--}27$ h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991)

Hydrolysis: first order hydrolysis $t_{1/2} = 2.8$ yr at pH 7 and 25°C, based on measured base rate constant; acid rate constant $k = 1.2 \times 10^{-7} \text{ M}^{-1}\cdot\text{h}^{-1}$ using measured rate constant for ethyl acrylate, resulting a $t_{1/2} = 280$ yr; base rate constant $k = 0.0779 \text{ M}^{-1}\cdot\text{h}^{-1}$ at pH 9 and 25°C with $t_{1/2} = 10$ d (Roy 1972; quoted, Howard et al. 1991).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on biological screening test data (Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.7\text{--}27$ h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991); atmospheric transformation lifetime was estimated to be < 1 to $1\text{--}5$ d (Kelly et al. 1994).

Surface water: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

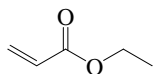
Groundwater: $t_{1/2} = 48\text{--}336$ h, based on measured hydrolysis data and estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

15.1.1.11 Ethyl acrylate



Common Name: Ethyl acrylate

Synonym: acrylic acid ethyl ester, ethyl 2-propenoate, propenoic acid ethyl ester

Chemical Name: ethyl acrylate, *n*-ethyl acrylate

CAS Registry No: 140-88-5

Molecular Formula: $C_5H_8O_2$, $CH_2=CHCOOCH_2CH_3$

Molecular Weight: 100.117

Melting Point ($^{\circ}C$):

−71.2 (Stull 1947; Weast 1982–83; Dean 1985; Riddick et al. 1986; Lide 2003)

Boiling Point ($^{\circ}C$):

99.4 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9234 (Weast 1982–83; Riddick et al. 1986)

0.9405 (Dean 1985)

Molar Volume (cm^3/mol):

109.2 (Stephenson & Malanowski 1987)

123.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

34.7 (at bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

20000 (Verschuereen 1983)

15000 (Dean 1985; Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

4860* (interpolated-regression of tabulated data, temp range -29.5 to $99.5^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 9259.4/(T/K)] + 8.347017$; temp range -29.5 to $99.5^{\circ}C$ (Antoine eq., Weast 1972–73)

3866, 6532 ($20^{\circ}C$, $30^{\circ}C$, Verschuereen 1983)

5100 (lit average, Riddick et al. 1986)

$\log(P/kPa) = 7.2103 - 1939.49/(T/K)$, temp range: not specified, (Antoine eq., Riddick et al. 1986)

5140 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_l/kPa) = 6.25041 - 1354.65/(-53.603 + T/K)$; temp range: 244–373 K (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 55.0109 - 3.5904 \times 10^3/(T/K) - 17.694 \cdot \log(T/K) + 8.051 \times 10^{-3} \cdot (T/K) - 4.8864 \times 10^{-13} \cdot (T/K)^2$; temp range 202–553 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ $25^{\circ}C$):

34.041 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

0.73 (Tute 1971; Laurence et al. 1972)

0.88 (calculated-fragment const. per Rekker 1977, Hermens & Leeuwangh 1982)

0.66 (HPLC-RT correlation, Fujisawa & Masuhara 1981)

1.33 (shake flask-GC, Tanii & Hashimoto 1982)

1.32 (recommended, Sangster 1989)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: photooxidation $t_{1/2} = 2.37\text{--}22.7$ h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: overall rate constant $k_h = 6.3 \times 10^{-9} \text{ s}^{-1}$ with $t_{1/2} = 3.5$ yr at 25°C and pH 7; acid rate constant $k_A = 1.2 \times 10^{-13} \text{ s}^{-1}$ and base rate constant $k_B = 7.8 \times 10^{-9} \text{ s}^{-1}$ at 25° and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 2.8$ yr at pH 7 and 25°C , based on acid and base catalyzed hydrolysis rate constants; acid rate constant $k_A = 1.2 \times 10^{-6} \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 244$ yr at pH 5; measured base rate constant $k_B = 0.078 \text{ M}^{-1} \cdot \text{h}^{-1}$ with $t_{1/2} = 10.4$ d at pH 9 and 25°C (Mabey & Mill 1978; quoted, Howard et al. 1991);

calculated rate constant for base-catalyzed hydrolysis $k_B = 5.0 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ and estimated $t_{1/2} \sim 25$ d in aqueous solutions at pH 8.8 (Freidig et al. 1999).

Biodegradation: aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on aqueous aerobic screening test data (Price et al. 1974; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 96\text{--}672$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 2.37\text{--}22.7$ h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Surface water: hydrolysis $t_{1/2} = 3.5$ yr at 25°C and pH 7 (Mabey & Mill 1978)

$t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 48\text{--}336$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 15.1.1.11.1
Reported vapor pressures of ethyl acrylate at various temperatures

Stull 1947	
summary of literature data	
$t/^\circ\text{C}$	P/Pa
−29.5	133.3
−8.70	666.6
2.0	1333
13.0	2666
26.0	5333
33.5	7999
44.5	13332
61.5	26664
80.0	53329
99.5	101325
mp/ $^\circ\text{C}$	−71.2

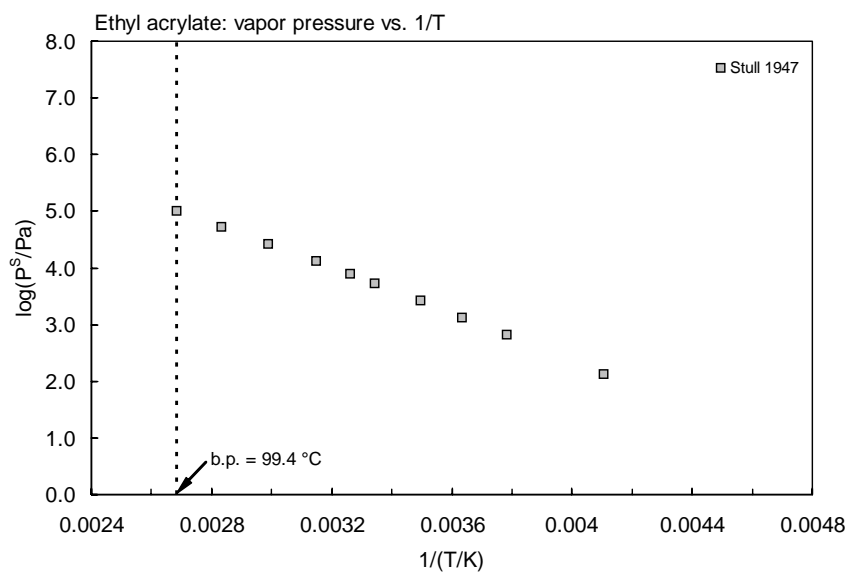
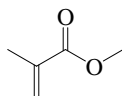


FIGURE 15.1.1.11.1 Logarithm of vapor pressure versus reciprocal temperature for ethyl acrylate.

15.1.1.12 Methyl methacrylate



Common Name: Methyl methacrylate

Synonym: methyl 2-methyl-2-propenoate, methyl ester methacrylic acid, methacrylic acid methyl ester, MMA

Chemical Name: 2-methyl-2-propenoic acid methyl ester

CAS Registry No: 80-62-6

Molecular Formula: $C_5H_8O_2$, $H_2C=C(CH_3)COOCH_3$

Molecular Weight: 100.117

Melting Point ($^{\circ}C$):

−47.55 (Lide 2003)

Boiling Point ($^{\circ}C$):

100.5 (Lide 2003)

Flash Point ($^{\circ}C$): 10

Density (g/cm^3 at $20^{\circ}C$):

0.9440 (Weast 1982–83)

Molar Volume (cm^3/mol):

106.6 ($25^{\circ}C$, Stephenson & Malanowski 1987)

121.8 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.7, 36.0 ($25^{\circ}C$, bp, Riddick et al. 1986)

Enthalpy of Fusion ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

16000 (Dean 1985)

15000 (USEPA 1985; ENVIROFATE; ISHOW)

15900 (Yalkowsky et al. 1987)

15600 ($20^{\circ}C$, Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

5332*, 4888 ($25.5^{\circ}C$, interpolated-regression of tabulated data, temp range -30.5 to $101^{\circ}C$, Stull 1947)

1315* ($3.44^{\circ}C$, temp range -45.26 to $3.44^{\circ}C$, Bywater 1952; quoted, Boublik et al. 1984)

$\log(P/mmHg) = [-0.2185 \times 8794.9/(T/K)] + 8.140942$; temp range -30.5 to $101^{\circ}C$ (Antoine eq., Weast 1972–73)

3732, 5333 ($20^{\circ}C$, $26^{\circ}C$, Verschuere 1977, 1983)

7003* ($32.489^{\circ}C$, temp range 32.489 – $99.855^{\circ}C$, Boublik & Aim 1979; quoted, Boublik et al. 1984)

5333 ($25.5^{\circ}C$, Weast 1982–83)

4440 (extrapolated average-Antoine eq., Boublik et al. 1984)

$\log(P/kPa) = 3.20496 - 4017.882/(126.685 + t/^{\circ}C)$; temp range -45.26 to $3.44^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

$\log(P/kPa) = 6.19400 - 1315.670/(213.490 + t/^{\circ}C)$; temp range: 32.41 – $99.855^{\circ}C$ (Antoine eq. from reported exptl. data, Boublik et al. 1984)

4846 (extrapolated-Antoine equation, Dean 1985)

$\log(P/mmHg) = 8.4092 - 2050.5/(274.4 + t/^{\circ}C)$; temp range: 39 – $89^{\circ}C$ (Antoine eq., Dean 1985, 1992)

5100 (lit. average, Riddick et al. 1986)

$\log(P/kPa) = 7.83859 - 2126.21/(T/K)$, temp range 0 – $30^{\circ}C$ (Antoine eq., Riddick et al. 1986)

5081, 5020 (interpolated-Antoine eq.-I and II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.63751 - 1597.9/(-28.76 + T/K)$; temp range: 293 – 374 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.43088 - 1461.197/(-43.15 + T/\text{K})$; temp range: 293–373 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = 106.896 - 5.2741 \times 10^3/(T/\text{K}) - 37.654 \cdot \log(T/\text{K}) + 1.862 \times 10^{-2} \cdot (T/\text{K}) - 3.6507 \times 10^{-13} \cdot (T/\text{K})^2$;
temp range 225–564 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

24.31 (calculated-P/C, USEPA 1985)
32.823 (calculated-P/C, Howard 1989)
32.09 (calculated-P/C, this work)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

0.73 (Tute 1971; Laurence et al. 1972)
0.70 (shake flask, Fujisawa & Masuhara 1981)
0.67 (HPLC-RT correlation, Fujisawa & Masuhara 1981)
1.36 (CLOGP, Hansch & Leo 1982)
1.38 (shake flask-GC, Tanii & Hashimoto 1982)
0.79 (calculated-f const. as per Lyman et al. 1982, USEPA 1985)
1.38 (recommended, Sangster 1989)
1.38 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

−0.03 (correlated as per Veith et al. 1979 for aquatic organisms, USEPA 1985)
0.55 (calculated- K_{OW} , Howard 1989)

Sorption Partition Coefficient, $\log K_{OC}$:

1.80 (calculated- K_{OW} as per Lyman et al. 1982, USEPA 1985)
1.94 (calculated- K_{OW} , Howard 1989)
0.74 (calculated- K_{OW} , Kollig 1993)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 6.3$ h from model river water (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: photodegradation $t_{1/2} = 2.7$ h in air of urban areas and $t_{1/2} > 3$ h in rural areas (Joshi et al. 1982; quoted, Howard 1989) (CHEMFATE; Hazardous Substance Databank).

Oxidation: photooxidation $t_{1/2} = 1.1$ –9.7 h in air, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991).

Hydrolysis: alkaline hydrolysis rate constant at 25°C, $k = 171 \text{ M}^{-1} \text{ h}^{-1}$ (Sharma & Sharma 1970; quoted, Ellington et al. 1987; Ellington 1989);

alkaline catalyzed rate constant $k(\text{exptl}) = 200 \text{ M}^{-1} \cdot \text{h}^{-1}$ at 25°C with estimated $t_{1/2} \sim 3.9$ yr at pH 7 and $t_{1/2} = 14$ d at pH 9 (Ellington et al. 1987; quoted, Ellington 1989; Howard 1989; Howard et al. 1991; Kollig 1993);

hydrolysis $t_{1/2} = 4$ yr at pH 7 and 25°C; base rate constant $k = 200 \text{ M}^{-1} \text{ h}^{-1}$ with $t_{1/2} = 14.4$ d at pH 9 based on measured rate constant at 25°C and pH 11 (Howard et al. 1991)

$k(\text{calc}) = 9.0 \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$, $2.6 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ for neutral and base-catalyzed hydrolysis and estimated $t_{1/2} \sim 8$ d in aqueous solutions at pH 8.8 (Freidig et al. 1999)

Biodegradation: completely degraded by activated sludge in approximately 20 h (Slave et al. 1974; quoted, EPA 1985; Howard 1989; Hazardous Substance Databank);

expert systems survey found that both aerobic ultimate degradation in receiving waters and anaerobic ultimate degradation were within a month and aerobic primary degradation in receiving waters was within few days (Boethling et al. 1989);

aqueous aerobic $t_{1/2} = 168$ –672 h, based on unacclimated screening test data (Pahren & Bloodgood 1961; Sasaki 1978; quoted, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672$ –2688 h, based on unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: photooxidation $t_{1/2} = 1.1\text{--}9.7$ h, based on estimated rate constants for the vapor phase reaction with hydroxyl radical (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be < 1 to $1\text{--}5$ d (Kelly et al. 1994).

Surface water: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Groundwater: $t_{1/2} = 336\text{--}1344$ h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: $t_{1/2} = 168\text{--}672$ h, based on estimated aqueous unacclimated aerobic biodegradation half-life (Howard et al. 1991).

Biota:

TABLE 15.1.1.12.1

Reported vapor pressures of methyl methacrylate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
Stull 1947		Bywater 1952		Boublik & Aim 1979	
summary of literature data		in Boublik et al. 1984		in Boublik et al. 1984	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
-30.5	133.3	-45.26	17	32.489	7003
-10.0	666.6	-43.46	25	37.962	9160
1.0	1333	-40.16	43	38.307	9306
11.0	2666	-35.16	64	43.731	12004
25.5	5333	-32.06	95	43.834	12049
34.5	7999	-27.96	140	47.951	14515
47.0	13332	-22.96	223	48.225	14680
63.0	26664	-20.46	260	53.954	18815
82.0	53329	-16.76	347	53.289	18290
101.0	101325	-10.56	547	55.846	20379
		-3.46	893	61.670	25849
mp/ $^{\circ}\text{C}$	-	-0.16	1053	65.350	29910
		3.44	1315	69.772	35421
				74.142	41676
		in Boublik et al. 1984		79.113	49831
		eq. 2	P/kPa	84.938	61430
		A	3.20496	91.998	77126
		B	401.882	99.855	98890
		C	126.685		
		bp/ $^{\circ}\text{C}$	-1.292	in Boublik et al. 1984	
		at 1 mmHg		eq. 2	P/kPa
				A	6.19400
				B	1315.670
				C	215.490
				bp/ $^{\circ}\text{C}$	100.641

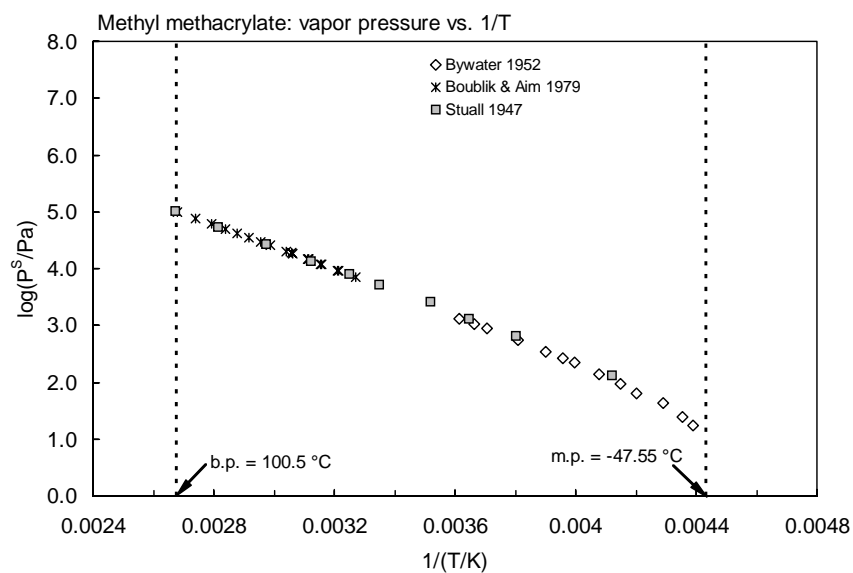
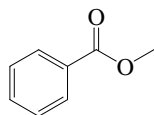


FIGURE 15.1.1.12.1 Logarithm of vapor pressure versus reciprocal temperature for methyl methacrylate.

15.1.2 AROMATIC ESTERS

15.1.2.1 Methyl benzoate



Common Name: Methyl benzoate

Synonym: benzoic acid methyl ester

Chemical Name: methyl benzoate

CAS Registry No: 93-58-3

Molecular Formula: $C_8H_8O_2$, $C_6H_5COOCH_3$

Molecular Weight: 136.149

Melting Point ($^{\circ}C$):

-12.4 (Lide 2003)

Boiling Point ($^{\circ}C$):

199 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.08854, 1.08377 ($20^{\circ}C$, $25^{\circ}C$, Dreisbach 1955)

Molar Volume (cm^3/mol):

125.0 (Stephenson & Malanowski 1987)

151.2 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

41.18, 55.84 (normal bp, $25^{\circ}C$, Dreisbach 1955)

43.18, 55.568 (normal bp, $25^{\circ}C$, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

9.736 (Dreisbach 1955; Riddick et al. 1986)

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

1524 (titration, Booth & Everson 1948)

4018 (Hine & Mookerjee 1975)

2100 ($20^{\circ}C$, quoted, Riddick et al. 1986)

1600 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

2130*, 2820 ($20.1^{\circ}C$, $29.6^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.5^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 7.48253 - 1974.6/(230 + t/^{\circ}C)$ (Antoine eq., Dreisbach & Martin 1949)

52.58 (calculated by formula, Dreisbach 1955)

$\log (P/mmHg) = 7.07832 - 1656.25/(195.23 + t/^{\circ}C)$; temp range: 100 – $260^{\circ}C$ (Antoine eq. for liquid state, Dreisbach 1955)

$\log (P/mmHg) = [-0.2185 \times 12077.2/(T/K)] + 8.509910$; temp range: 39 – $199.5^{\circ}C$ (Antoine eq., Weast 1972–73)

77.6 (extrapolated-Antoine eq., Dean 1985)

$\log (P/mmHg) = 6.60743 - 1974.6/(230.0 + t/^{\circ}C)$; temp range 111 – $199^{\circ}C$ (Antoine eq., Dean 1985, 1992)

52.58 (quoted lit. average, Riddick et al. 1986)

$\log (P/kPa) = 6.60743 - 1974.6/(230 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

54.5 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 8.183 - 2816.6/(T/K)$; temp range 283 – $323 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/\text{kPa}) = 6.20322 - 1656.25/(-77.92 + T/\text{K})$; temp range: 383–533 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/\text{mmHg}) = -13.6342 - 2.9133 \times 10^3/(T/\text{K}) + 11.773 \cdot \log (T/\text{K}) - 2.3979 \times 10^{-2} \cdot (T/\text{K}) + 1.1324 \times 10^{-5} \cdot (T/\text{K})^2$;
temp range 261–693 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 1.80 (calculated- C_w/C_A , Hine & Mookerjee 1975)
- 2.48 (calculated-bond contribution, Hine & Mookerjee 1975)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 2.15 (HPLC-RT correlation, D'Amboise & Hanai 1982)
- 2.22 (HPLC- k' correlation, Haky & Young 1984)
- 2.14 (shake flask-HPLC, Nielson & Bundgaard 1988)
- 2.10 (recommended, Klein et al. 1988)
- 2.15 (RP-HPLC-RT correlation, ODS column with masking agent, Bechalany et al. 1989)
- 2.20 (recommended, Sangster 1989)
- 2.12 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.30, 2.01, 1.98 (Podzol soil, Alfisol soil, sediment, von Oepen et al. 1991)
- 1.89 (calculated-MCI χ , Meylan et al. 1992)
- 2.10 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 2.14; 2.57, 2.14, 1.94, 2.16, 1.89 (soil: calculated- K_{ow} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: overall rate constant $k_h = 1.90 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 118 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)
alkaline hydrolysis rate constant $k = 0.0794 \text{ M}^{-1} \text{ s}^{-1}$ (Drossman et al. 1988, quoted, Collette 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants::

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 118 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.2.1.1

Reported aqueous solubilities of methyl benzoate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC

$t/^{\circ}\text{C}$	$S/\text{g}\cdot\text{m}^{-3}$
0	2210
9.7	2210
20.1	2130
29.6	2820
40.2	2470
49.8	2580
60.1	2860
70.2	3250
80.3	3580
90.5	4080

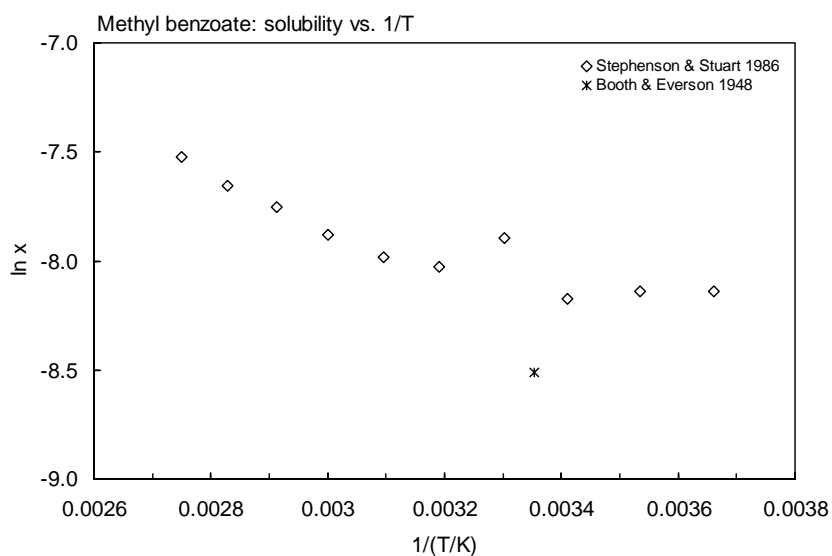
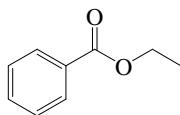


FIGURE 15.1.2.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for methyl benzoate.

15.1.2.2 Ethyl benzoate



Common Name: Ethyl benzoate

Synonym: benzoic acid ethyl ester, ethyl benzenecarboxylate

Chemical Name: benzoic acid ethyl ester, ethyl benzenecarboxylate, ethyl benzoate

CAS Registry No: 93-89-0

Molecular Formula: $C_9H_{10}O_2$, $C_6H_5COOC_2H_5$

Molecular Weight: 150.174

Melting Point ($^{\circ}C$):

−34 (Lide 2003)

Boiling Point ($^{\circ}C$):

212 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0468 (Weast 1982–83)

1.0511, 1.0372 ($15^{\circ}C$, $30^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

175.0 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

40.5 (Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

720 (Seidell 1941; quoted, Andrews & Keefer 1950)

598 (Deno & Berkheimer 1960)

702 (calculated- K_{ow} , Hansch et al. 1968)

510 (calculated- K_{ow} , Yalkowsky & Morozowich 1980)

2026 (calculated- K_{ow} and mp, Amidon & Williams 1982),

807 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

1090 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Kamlet et al. 1987)

464 (calculated-intrinsic molar volume V_1 and mp, Kamlet et al. 1987)

500 ($20^{\circ}C$, Riddick et al. 1986)

926 (calculated-fragment const., Wakita et al. 1986)

398 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

850*, 810 ($19.6^{\circ}C$, $30^{\circ}C$, shake flask-GC/TC, measured range 0 – $90.3^{\circ}C$, Stephenson & Stuart 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

42.1 (extrapolated-regression of tabulated data, temp range 44 – $213.4^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 11981.5/(T/K)] + 8.279591$; temp range 44 – $213.4^{\circ}C$ (Antoine eq., Weast 1972–73)

24.0 ($20^{\circ}C$, quoted lit., Riddick et al. 1986)

$\log(P/kPa) = 7.7579 - 2750.0/(T/K)$; temp range 90 – $140^{\circ}C$ (Antoine eq., Riddick et al. 1986)

$\log(P/kPa) = 7.1599 - 2500.0/(T/K)$; temp range 140 – $220^{\circ}C$ (Antoine eq., Riddick et al. 1986)

27.5 (interpolated-Antoine eq.-II, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 6.81152 - 2174.3/(-34.071 + T/K)$; temp range 358 – $487 K$ (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 8.23958 - 2922.167/(T/K)$; temp range 288 – $333 K$ (Antoine eq.-II, Stephenson & Malanowski 1987)

$$\log (P/\text{mmHg}) = 40.8047 - 3.9985 \times 10^3/(T/K) - 11.793 \cdot \log (T/K) + 4.0697 \times 10^{-3} \cdot (T/K) - 1.2372 \times 10^{-13} \cdot (T/K)^2;$$

temp range 238–698 K (vapor pressure eq., Yaws 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

10.298 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

2.62 (calculated, Hansch et al. 1968)
 2.20 (shake flask-spectrophotometry, Yaguzhinskii et al. 1973)
 2.64 (Valvani et al. 1981, Amidon & Williams 1982)
 2.64 (shake flask-HPLC, Nielsen & Bundgaard 1988)
 2.60 (recommended, Klein et al. 1988)
 2.64 (recommended, Sangster 1989)
 2.66, 2.89, 2.90 (centrifugal partition chromatography CPC-RV, Gluck & Martin 1990)
 2.70 ± 0.15 , 2.63 ± 0.57 (solvent generated liquid-liquid chromatography SGLLC-correlation, RP-HPLC- k' correlation, Cichna et al. 1995)
 2.64 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{oc}$:

2.25, 2.17, 2.43 (sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
 2.16 (calculated-MCI χ and fragment contribution, Meylan et al. 1992)
 2.30 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: overall rate constant $k_h = 3.0 \times 10^{-9} \text{ s}^{-1}$ with $t_{1/2} = 7.3 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

alkaline hydrolysis rate constant $k = 0.0316 \text{ M}^{-1} \text{ s}^{-1}$ (Drossman et al. 1988, quoted, Collette 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 7.3 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.2.2.1

Reported aqueous solubilities of ethyl benzoate at various temperatures

Stephenson & Stuart 1986

shake flask-GC/TC	
t/°C	S/g·m ⁻³
0	1080
19.6	850
30.5	810
40.0	1060
50.0	1080
60.1	1170
70.5	1210
80.2	1210
90.3	1430

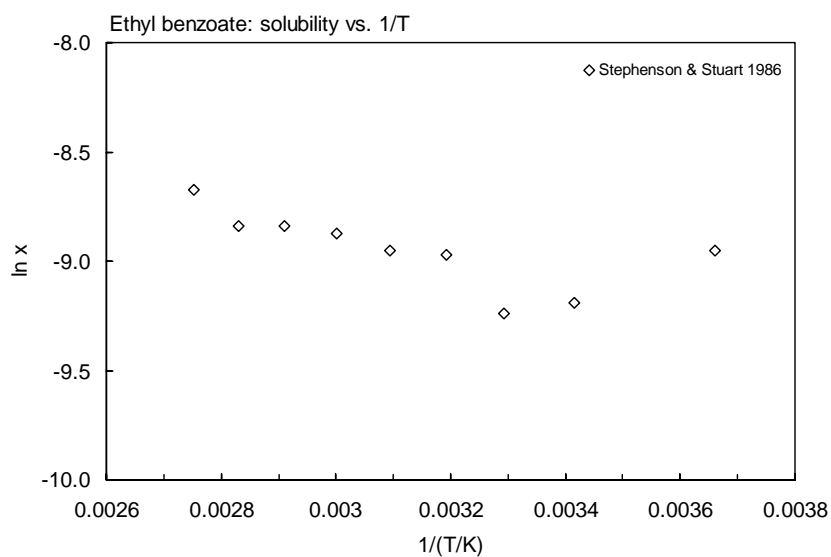
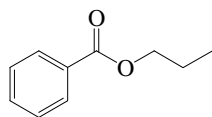


FIGURE 15.1.2.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for ethyl benzoate.

15.1.2.3 *n*-Propyl benzoate

Common Name: *n*-Propyl benzoate

Synonym: benzoic acid *n*-propyl ester, propyl benzenecarboxylate

Chemical Name: benzoic acid *n*-propyl ester, propyl benzenecarboxylate, propyl benzoate

CAS Registry No: 2315-68-6

Molecular Formula: $C_{10}H_{12}O_2$, $C_6H_5COOCH_2CH_2CH_3$

Molecular Weight: 164.201

Melting Point ($^{\circ}C$):

−51.6 (Weast 1982–83; Riddick et al. 1986; Stephenson & Malanowski 1987; Lide 2003)

Boiling Point ($^{\circ}C$):

211 (Weast 1982–83; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0232 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

160.5 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

199.4 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

51.92; 49.75 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

350 (quoted exptl., Kamlet et al. 1987)

292 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Kamlet et al. 1987)

140 (calculated-intrinsic molar volume V_1 and mp, Kamlet et al. 1987)

966 (calculated-MCI χ , Nirmalakhandan & Speece 1988)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations):

133.3 ($54.6^{\circ}C$, summary of literature data, temp range 54.6 – $231^{\circ}C$, Stull 1947)

$\log(P/mmHg) = [-0.2185 \times 12318.7/(T/K)] + 8.237827$; temp range 54.6 – $231^{\circ}C$ (Antoine eq., Weast 1972–73)

100 ($54.6^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 7.42756 - 2172.71/(T/K)$; temp range 80 – $160^{\circ}C$ (Antoine eq., Riddick et al. 1986)

$\log(P_L/kPa) = 6.68614 - 2165.28/(-41.593 + T/K)$; temp range 327 – 504 K (Antoine eq., Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.80 (shake flask-HPLC, Nielsen & Bundgaard 1988)

3.18 (recommended, Sangster 1989)

3.01 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

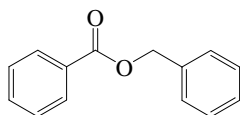
Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Half-Lives in the Environment:

15.1.2.4 Benzyl benzoate



Common Name: Benzyl benzoate

Synonym: benzoic acid benzyl ester, phenylmethyl benzoate, benzyl benzenecarboxylate, benzyl phenylformate, benzenoate

Chemical Name: benzyl benzoate, phenylmethyl benzoate, benzyl benzenecarboxylate

CAS Registry No: 120-51-4

Molecular Formula: $C_{14}H_{12}O_2$, $C_6H_5COOCH_2C_6H_5$

Molecular Weight: 212.244

Melting Point ($^{\circ}C$):

19.4 (Riddick et al. 1986)

Boiling Point ($^{\circ}C$):

323.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.1121 ($25^{\circ}C$, Weast 1982–83)

1.120, 1.1121 ($19.5^{\circ}C$, $25^{\circ}C$, Riddick et al. 1986)

Molar Volume (cm^3/mol):

190.9 ($25^{\circ}C$, calculated-density)

243.6 (calculated-Le Bas method at normal boiling point)

Dissociation Constant, pK_a :

Enthalpy of Vaporization, ΔH_v (kJ/mol):

53.56 (at normal bp, Hon et al. 1976)

77.8; 53.6 ($25^{\circ}C$; bp, Riddick et al. 1986)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

15.73 (Seidell 1941; quoted, Deno & Berkheimer 1960)

61.21 (calculated-intrinsic molar volume V_1 and solvatochromic parameters, Leahy 1986)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log (P/mmHg) = 6.42726 - 1594.49/(126.36 + t/^{\circ}C)$; temp range $224.7-329.09^{\circ}C$ (Antoine eq., from twin ebulliometry measurement, Hon et al. 1976)

0.0137 (extrapolated-Antoine eq., Boublik et al. 1984)

$\log (P/kPa) = 5.59354 - 1628.726/(130.735 + t/^{\circ}C)$; temp range $224.7-329^{\circ}C$ (Antoine eq. from reported exptl. data of Hon et al. 1976, Boublik et al. 1984)

461 ($150^{\circ}C$, quoted lit., Riddick et al. 1986)

0.0104 (calculated-Antoine eq., Riddick et al. 1986)

$\log (P/kPa) = 5.55216 - 1594.49/(126.36 + t/^{\circ}C)$; temp range not specified (Antoine eq., Riddick et al. 1986)

0.043 (interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 9.240 - 4057/(T/K)$; temp range 297–353 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log (P_L/kPa) = 5.63847 - 1666.706/(-137.564 + T/K)$; temp range 497–602 K (Antoine eq.-II, Stephenson & Malanowski 1987)

$\log (P/mmHg) = -1.654 - 4.6284 \times 10^3/(T/K) + 7.363 \cdot \log (T/K) - 1.8259 \times 10^{-2} \cdot (T/K) + 7.4580 \times 10^{-6} \cdot (T/K)^2$; temp range 293–820 K (vapor pressure eq., Yaws et al. 1994)

0.0178, 0.0107, 0.0135, 0.295, 0.0603 (GC-RT correlation, Sugden's parachor method, McGowan's parachor method, calculated-MCI, calculated-MW, Tsuzuki 2001)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

0.57 (calculated-P/C with selected values)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

3.86 (quoted, calculated- V_I and solvatochromic parameters, Taft et al. 1985)

4.00 (quoted, calculated- V_I and solvatochromic parameters, Leahy 1986)

3.97 (recommended value, Sangster 1989)

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Hydrolysis:

Oxidation:

Hydrolysis: overall rate constant $k_h = 8.0 \times 10^{-10} \text{ s}^{-1}$ with $t_{1/2} = 27 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

alkaline hydrolysis rate constant $k = 0.00794 \text{ M}^{-1} \text{ s}^{-1}$ (Mabey et al. 1978; quoted, Collette 1990)

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolysis $t_{1/2} = 27 \text{ yr}$ at 25°C and pH 7 (Mabey & Mill 1978)

Groundwater:

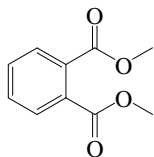
Sediment:

Soil:

Biota:

15.1.3 PHTHALATE ESTERS

15.1.3.1 Dimethyl phthalate (DMP)



Common Name: Dimethyl phthalate

Synonym: DMP, 1,2-benzenedicarboxylic acid dimethyl ester, dimethyl-1,2-benzenedicarboxylate, methyl Common phthalate, *o*-dimethylphthalate, phthalic acid dimethyl ester

Chemical Name: dimethyl phthalate, dimethyl-*o*-phthalate, methyl phthalate

CAS Registry No: 131-11-3

Molecular Formula: $C_{10}H_{10}O_4$, $o\text{-C}_6\text{H}_4(\text{COOCH}_3)_2$

Molecular Weight: 194.184

Melting Point ($^{\circ}\text{C}$):

5.5 (Lide 2003)

Boiling Point ($^{\circ}\text{C}$):

283.7 (Lide 2003)

Density (g/cm^3 at 20°C):

1.189 (25°C , Fishbein & Albro 1972)

1.1905 (20°C , Weast 1982–83)

Molar Volume (cm^3/mol):

162.8 (calculated-density, Stephenson & Malanowski 1987)

206.4 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

78.66 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($\text{J}/\text{mol K}$):

Fugacity Ratio at 25°C (assuming $\Delta S_{\text{fus}} = 56 \text{ J}/\text{mol K}$) F: 1.0

Water Solubility (g/m^3 or mg/L at 25°C or as indicated and reported temperature dependence equations):

3965 (Deno & Berkheimer 1960)

5000 (20°C , Fishbein & Albro 1972)

4000 (32°C , from Monsanto Chemical Co. data sheets, Peakall 1975)

4320 ± 37 (shake flask-GC, Wolfe et al. 1980b; Wolfe et al. 1980a)

4248 (shake flask-LSC, Veith et al. 1980)

4290 (20°C , shake flask-UV, Leyder & Boulanger 1983)

5000, 1744 (20°C , Verschueren 1983)

4000 ± 60 (shake flask-HPLC/UV, Howard et al. 1985)

2810 (21°C , shake flask-HPLC/UV, Nielsen & Bundgaard 1989)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

40* (82°C , ebulliometry, measured range $82\text{--}151^{\circ}\text{C}$, Gardner & Brewer 1937)

$\log (P/\text{mmHg}) = 9.117 - 1496.375/(T/K)$; temp range $82\text{--}151^{\circ}\text{C}$ (Antoine eq. derived by Kim 1985 from exptl data of Gardner & Brewer 1937)

0.863* (extrapolated-regression of tabulated data, temp range $100.3\text{--}288.7^{\circ}\text{C}$ Stull 1947)

0.245 (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log (P/\text{mmHg}) = 11.06 - 4113/(T/K)$; temp range $32\text{--}55^{\circ}\text{C}$ or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948)

0.559 (20°C , calculated-Antoine eq., Weast 1972–73)

$\log (P/\text{mmHg}) = [-0.2185 \times 14922.2/(T/K)] + 8.747053$; temp range $100.3\text{--}287^{\circ}\text{C}$ (Antoine eq., Weast 1972–73)

0.445 (gas saturation, extrapolated, measured range $60\text{--}100^{\circ}\text{C}$, Potin-Gautier et al. 1982)

$\log (P/\text{mmHg}) = 8.899 - 3332.764/(T/K)$; temp range 60–100°C (Antoine eq., Potin-Gautier et al. 1982)
 $\log (P/\text{kPa}) = 3.64598 - 699.876/(51.372 + t/^{\circ}\text{C})$; temp range 82–151°C (Antoine eq. from reported exptl. data, Boublik et al. 1984)
 $\log (P/\text{mmHg}) = 4.52232 - 700.31/(51.42 + t/^{\circ}\text{C})$; temp range 82–151°C (Antoine eq., Dean 1985, 1992)
 0.220 (gas saturation-HPLC/UV, Howard et al. 1985; quoted, Howard et al. 1986; Howard 1989; Banerjee et al. 1990)
 0.245, 0.863 (extrapolated-Antoine eq.-I, II, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 10.185 - 4113/(T/K)$; temp range 304–371 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log (P_L/\text{kPa}) = 8.095 - 3327/(T/K)$; temp range 371–547 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 1.190 (GC-RT correlation, Hinckley et al. 1990)
 $\log (P/\text{mmHg}) = 12.6974 - 4.1989 \times 10^3/(T/K) + 0.3463 \cdot \log(T/K) - 7.6524 \times 10^{-3} \cdot (T/K) + 3.349 \times 10^{-6} \cdot (T/K)^2$;
 temp range 272–766 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($\text{Pa m}^3/\text{mol}$ at 25°C):

0.111 (calculated-P/C, Fishbein & Albro 1972)
 0.111 (calculated-P/C, Wolfe et al. 1980a)
 0.011 (calculated as per Lyman et al. 1982; quoted, Howard 1989)
 0.218 (20°C, calculated-P/C, Mabey et al. 1982)
 0.012 (selected, Staples et al. 1997)
 0.00978 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

1.61 (shake flask-LSC, Veith et al. 1980; Veith & Kosian 1983)
 1.56 (HPLC-RT correlation, Veith et al. 1980)
 1.62, 1.82 (HPLC- k' correlations, McDuffie 1981)
 1.53 (20°C, shake flask-UV, Leyder & Boulanger 1983)
 1.47, 1.90 (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)
 1.56 (shake flask, unpublished data, Hansch & Leo 1985; 1987)
 1.66 (shake flask, average from interlaboratory study, Renberg et al. 1985)
 1.74, 1.61 (HPLC, RP-TLC, average from interlaboratory study, Renberg et al. 1985)
 1.62 (HPLC-RT correlation, Eadsforth 1986)
 1.46 (shake flask-HPLC/UV, Nielsen & Bundgaard 1989)
 1.56 (recommended, Sangster 1993)
 1.56 (recommended, Hansch et al. 1995)
 1.61 (recommended, Staples et al. 1997)
 1.54 (micro-emulsion electrokinetic chromatography-retention factor correlation, Poole et al. 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.01 (calculated-QSPR, Cousin & Mackay 2000)

Bioconcentration Factor, $\log \text{BCF}$:

0.67 (calculated- K_{OW} , Veith et al. 1979, 1980)
 1.76 (bluegill sunfish, Barrows et al. 1980)
 1.76 (bluegill sunfish, Veith et al. 1980; Veith & Kosian 1983)
 1.42 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
 0.49–0.8, 0.67–0.78 (shrimp, fish, Wofford et al. 1981)
 1.20 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
 0.77 (sheepshead minnow, quoted from Wofford et al. 1981, Zaroogian et al. 1985)
 1.76, 2.22 (quoted, calculated-MCI χ , Sabljic 1987)
 0.67, 0.73 (brown shrimp, sheepshead minnow, quoted, Howard 1989)
 1.76 (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

1.64 (soil, estimated, Kenaga 1980)
 2.20 (soil, estimated- K_{OW} , Wolfe et al. 1980a)

- 1.74 (soil/sediment, Osipoff et al. 1981)
 1.24 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 1.52 (sediment, calculated- K_{OW} , Pavlou & Weston 1983, 1984)
 2.69 (activated carbon, calculated- MCI χ , Blum et al. 1994)
 1.20 (calculated- K_{OW} , Kollig 1993)
 1.60 (quoted or calculated-QSAR MCI χ , Sabljic et al. 1995)
 4.70 (suspended solids, calculated- K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)
 1.64, 2.14; 2.16, 1.87, 2.53, 1.83, 1.67 (soil: quoted lit., calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constant, k , and Half-Lives $t_{1/2}$:

Volatilization: estimated $t_{1/2} = 46$ d from a river of 1 m deep with 1.0 m/s current and a 3.0 m/s wind using calculated Henry's law constant and considering the volatilization rate being controlled by the diffusion through the air layer (Lyman et al. 1982; quoted, Howard 1989).

Photolysis: direct $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a);

abiotic degradation $t_{1/2} = 3500$ h for direct sunlight in surface waters and $t_{1/2} = 12.7$ h in pure water but reduced to 2.8 h in the presence of NO_2 when irradiated with a UV lamp through a Pyrex filter (Howard 1989)

Indirect photolysis rate $k = 0.048 \text{ d}^{-1}$ with $t_{1/2} = 14.4$ d in air (Peterson & Staples 2003)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(\text{aq.}) = 18 \text{ M}^{-1} \text{ s}^{-1}$ for reaction with free radical in aqueous environment (Wolfe et al. 1980a)

$k(\text{aq.}) \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $0.05 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

photooxidation $t_{1/2} = 23.8$ h (estimated, Howard 1989)

atmospheric $t_{1/2} = 112\text{--}1118$ h, based on estimated rate data for the reaction with OH radical in air (Howard et al. 1991)

$k(\text{aq.}) = (0.20 \pm 0.10) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $21 \pm 1^\circ\text{C}$, with a $t_{1/2} = 1.9$ d at pH 7 (Yao & Haag 1991).

$k(\text{aq.}) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

photooxidation $t_{1/2}(\text{predicted}) = 9.3\text{--}93$ d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)

$k_{OH} = 5.74 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 14.4$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis: $k(\text{acid-catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{alkaline}) = 2.5 \times 10^2 \text{ M}^{-1} \text{ h}^{-1}$; phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4$ month to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)

$k(\text{second-order alkaline}) = 6.9 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 8 and 30°C , and $t_{1/2} = 4$ months for hydrolytic degradation in the eutrophic lake system (Wolfe et al. 1980b; quoted, Kollig 1993)

$k(\text{second-order alkaline}) = 6.9 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 10–12 and 30°C in water with $t_{1/2}(\text{calc}) = 3.2$ yr at pH 7 (Callahan et al. 1979)

hydrolysis half-lives: $t_{1/2} = 3.2$ yr under natural conditions at 30°C , $t_{1/2} = 11.6$ d at 30°C and $t_{1/2} = 25$ d at 18°C and at pH 9 (Howard 1989; selected, Staples et al. 1997);

first-order hydrolysis $t_{1/2} = 1163$ d based on a second-order rate constant at pH 7 and 30°C ; and a base rate constant $k = 111.6 \text{ M}^{-1} \text{ h}^{-1}$ corresponding to $t_{1/2} = 1.2$ d at pH 9 and 18°C (Howard et al. 1991)

$t_{1/2} = 1200$ d at pH 7, $t_{1/2} = 0.026$ d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation: calculated rate constant $k = (9.49 \pm 0.41) \times 10^2 \text{ min}^{-1}$ from retention times in reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985);

significant degradation with rapid adaption within 7 d in an aerobic environment with a rate $k > 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);

biodegradation rate constant $k = 1.2 \times 10^{-4} \text{ mL-cell}^{-1} \cdot \text{d}^{-1}$ in river die-away test (Scow 1982);

58–88% mineralization in 7 d in municipal digested sludge (Horowitz et al. 1982);

rate constant $k = 0.364 \text{ d}^{-1}$ which corresponds to $t_{1/2} = 1.90$ d in shake flask biodegradation experiments (Sugatt et al. 1984);

greater than 90% of DMP was degraded within 40 d in digested sludge (Shelton et al. 1984);

biodegraded in excess of 90% in activated sludge systems in less than 24 h (O'Grady et al. 1985);

soil-water biodegradation studies showed that 85% loss in Broome County soil after 120 hours and 75% loss in leachate sprayed soil after 48 h (Russell et al. 1985);

anaerobic digestion of sludge with a first-order $k = 8.9 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 78 \text{ h}$ (Ziogou et al. 1989); aqueous aerobic $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data; aqueous anaerobic $t_{1/2} = 96\text{--}672 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 3 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

$k = 0.0290 \text{ h}^{-1}$ with $t_{1/2} = 23.9 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000)

Aerobic biodegradation in aquatic environments, first order $k = 0.5 \text{ d}^{-1}$ with $t_{1/2} = 1.39 \text{ d}$ in river water, $k = 0.5 \text{ d}^{-1}$ with $t_{1/2} = 1.39 \text{ d}$ in MITI inoculum (Peterson & Staples 2003)

Aerobic biodegradation in soil, pseudo-first-order rate $k = 0.36 \text{ d}^{-1}$ with $t_{1/2} = 1.93 \text{ d}$ in agitated aqueous suspension, and $k = 0.40 \text{ d}^{-1}$ with $t_{1/2} = 1.70 \text{ d}$ at 30°C in garden soil. For anaerobic degradation, first order rate $k = 0.25\text{--}0.696 \text{ d}^{-1}$ with $t_{1/2} = 2.8\text{--}1.0 \text{ d}$ in digester sludge, batch incubation; $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21 \text{ d}$ in flood soil (Peterson & Staples 2003)

Biotransformation: estimated rate constant $k \sim 5.2 \times 10^{-6} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

depuration $t_{1/2} = 24\text{--}48 \text{ h}$ from bluegill sunfish (Barrows et al. 1980).

$k_2 = 27.7 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 2.37 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: atmospheric $t_{1/2} = 23.8 \text{ h}$ for reaction with hydroxyl radicals (Howard 1989);

$t_{1/2} = 112\text{--}1118 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

atmospheric transformation lifetime was estimated to be 1 to 5 d (Kelly et al. 1994).

$t_{1/2} = 14.41 \text{ d}$ based on photooxidation reaction rate with OH radical, indirect photolysis $t_{1/2} = 14.4 \text{ d}$ (Peterson & Staples 2003)

Surface water: estimated $t_{1/2} < 0.3 \text{ d}$ in river waters (Zoeteman et al. 1980);

mineralization $t_{1/2} \sim 7 \text{ d}$ in municipal digested sludge (Horowitz et al. 1982);

biodegradation $t_{1/2} = 1.90 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984);

$t_{1/2} < 192\text{--}264 \text{ h}$ by biodegradation in fresh river water, $t_{1/2} = 12 \text{ h}$ in Rhine River, an estimated $t_{1/2} \sim 13\text{--}27 \text{ h}$ in a modelling study of simulated ecosystem; abiotic degradation $t_{1/2} = 12.7 \text{ h}$ in pure water and $t_{1/2} = 2.8 \text{ h}$ in the presence of nitrogen dioxide when irradiated with a UV lamp (Howard 1989);

overall degradation $t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated river die-away test data (Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 4 \text{ d}$ in natural waters (Capel & Larson 1995)

$k(\text{exptl}) = (0.20 \pm 0.10) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and $21\text{--}1^\circ\text{C}$, with $t_{1/2} = 1.9 \text{ d}$ at pH 7 (Yao & Haag 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 4 \text{ d}$ and $t_{1/2} = 1200$ at pH 7, $t_{1/2} = 0.026 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

$t_{1/2} = 0.5\text{--}1.39 \text{ d}$ for biodegradation in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 48\text{--}336 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: biodegradation $t_{1/2} < 5 \text{ d}$ (aerobic) and $t_{1/2} \sim 20 \text{ d}$ (anaerobic) in a garden soil (Shanker et al. 1985);

$t_{1/2} = 10\text{--}50 \text{ d}$, via volatilization subject to plant uptake from soil (Ryan et al. 1988);

$t_{1/2} = 24\text{--}168 \text{ h}$, based on unacclimated aerobic river die-away test data and acclimated aerobic soil grab sample data (Howard et al. 1991)

Biodegradation in aerobic soil: $t_{1/2} = 1.93 \text{ d}$ in agitated aqueous suspension and $t_{1/2} = 1.70 \text{ d}$ in garden soil (Peterson & Staples 2003)

Biota: $24 < t_{1/2} < 48 \text{ h}$ depuration half-life in tissues of bluegill sunfish in 21 d-exposure experiment (Barrows et al. 1980; quoted, Howard 1989);

$t_{1/2} = 23.9 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000).

TABLE 15.1.3.1.1

Reported vapor pressures of dimethyl phthalate at various temperatures and the coefficients for the vapor pressure equations

$$\begin{aligned}\log P &= A - B/(T/K) & (1) & \quad \ln P = A - B/(T/K) & (1a) \\ \log P &= A - B/(C + t/^{\circ}\text{C}) & (2) & \quad \ln P = A - B/(C + t/^{\circ}\text{C}) & (2a) \\ \log P &= A - B/(C + T/K) & (3) & \\ \log P &= A - B/(T/K) - C \cdot \log (T/K) & (4) & \end{aligned}$$

Gardner & Brewer 1937		Stull 1947	
ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa
82.0	40.0	100.3	133.3
85.0	53.3	131.8	666.6
90.0	66.7	147.6	1333
99.0	80.0	164.0	2666
103.0	120	182.8	5333
105.3	160	194.0	7999
107.4	213	210.0	13332
110.6	227	232.7	26664
115.0	267	257.8	53329
118.0	333	283.7	101325
123.8	440		
129.5	587	mp/°C	
136.9	813		
146.5	1293		
146.9	1293		
150.6	1533		
151.0	1547		
bp/°C	140.586		
	at 1 mmHg		

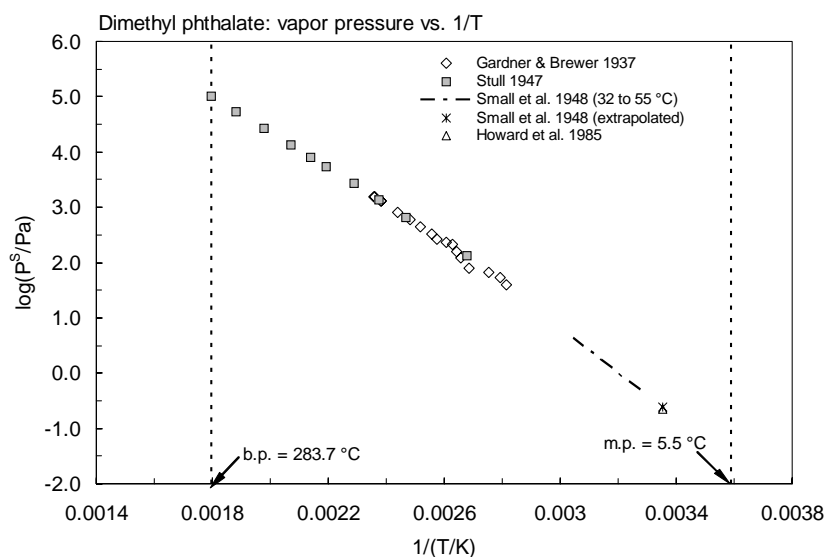
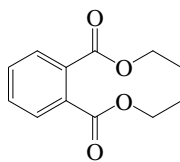


FIGURE 15.1.3.1.1 Logarithm of vapor pressure versus reciprocal temperature for dimethyl phthalate.

15.1.3.2 Diethyl phthalate (DEP)



Common Name: Diethyl phthalate

Synonym: DEP, ethyl phthalate

Chemical Name: phthalic acid diethyl ester, ethyl phthalate, 1,2-benzenedicarboxylic acid ethyl ester

CAS Registry No: 84-66-2

Molecular Formula: $C_{12}H_{14}O_4$, $C_6H_4(COOC_2H_5)_2$

Molecular Weight: 222.237

Melting Point ($^{\circ}C$):

−40.5 (Patty 1963; Fishbein & Albro 1972; Lide 2003)

Boiling Point ($^{\circ}C$):

295 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.123 ($25^{\circ}C$, Fishbein & Albro 1972)

1.1175 ($20^{\circ}C$, Weast 1982–83)

Molar Volume (cm^3/mol):

198.9 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

254.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

82.42 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$) F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

598 (Deno & Berkheimer 1960)

1000 ($20^{\circ}C$, Fishbein & Albro 1972)

1000 ($32^{\circ}C$, from Monsanto Chemical Co. data sheets, Peakall 1975)

896 (shake flask-GC, Wolfe et al. 1980b)

1200* ($20^{\circ}C$, elution chromatography, UV, Schwarz & Miller 1980)

7028 (shake flask-LSC, Veith et al. 1980)

928 ($20^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

1080 (shake flask-HPLC/UV, Howard et al. 1985)

680 (measured, Russell & McDuffie 1986)

938* (shake flask-surface tension measurement, measured range 10 – $35^{\circ}C$ Thomsen et al. 2001)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.467* (extrapolated-regression of tabulated data, temp range 108.8 – $294^{\circ}C$, Stull 1947)

0.086 (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log(P/mmHg) = 11.26 - 4308/(T/K)$; temp range 32 – $60^{\circ}C$ or pressure range 5×10^{-2} to 10^{-4} mmHg (effusion method, data presented in graph and Antoine eq., Small et al. 1948)

0.052 ($20^{\circ}C$, torsion-effusion method, Balson 1958)

0.0195 ($20^{\circ}C$, aerosol saturation, measured range 25 – $70^{\circ}C$, Frostling 1970)

$\log(P/mmHg) = 11.13 - 4275/(T/K)$; temp range 25 – $70^{\circ}C$ (aerosol saturation, Frostling 1970)

0.467 (calculated-Antoine eq., Weast 1972–73)

$\log(P/mmHg) = [-0.2185 \times 15383.0/(T/K)] + 8.18275$; temp range 108.8 – $294^{\circ}C$ (Antoine eq., Weast 1972–73)

- 0.046* (20°C, extrapolated, gas-saturation method, measured range 34.2–60.5°C, Grayson & Fosbraey 1982)
 $\ln(P/\text{Pa}) = 32.50 - 10436/(T/\text{K})$; temp range 34.2–60.5°C (Antoine eq., gas saturation-GC, Grayson & Fosbraey 1982)
- 1.867 (gas saturation, measured range 60–120°C. Potin-Gautier et al. 1982)
 $\log(P/\text{mmHg}) = 8.806 - 1443.039/(T/\text{K})$; temp range 60–120°C (Potin-Gautier et al. 1982)
- 0.220 (gas saturation-HPLC/UV, Howard et al. 1985)
- 0.0064 (extrapolated-Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.04308 - 1866.05/(-115.9 + T/\text{K})$; temp range 345–453 K (Antoine eq.-I, Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 10.6902 - 6768.3/(-209.45 + T/\text{K})$; temp range 421–570 K (Antoine eq.-II, Stephenson & Malanowski 1987)
- 0.280 (GC-RT correlation, Hinckley et al. 1990)
 $\log(P/\text{mmHg}) = 72.1438 - 7.0747 \times 10^3/(T/\text{K}) - 21.029 \cdot \log(T/\text{K}) - 3.2404 \times 10^{-10} \cdot (T/\text{K}) + 3.4691 \times 10^{-6} \cdot (T/\text{K})^2$;
 temp range 269–757 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.0020 (calculated-P/C, Wolfe et al. 1980a)
- 0.0486 (Lyman et al. 1982; quoted, Howard 1989)
- 0.1220 (calculated-P/C, Mabey et al. 1982)
- 4.7100 (quoted from WERL Treatability Data, Ryan et al. 1988)
- 0.0269 (selected, Staples et al. 1997)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 3.22 (calculated as per Leo et al. 1971)
- 3.15 (RP-HPLC-RT correlation, Veith et al. 1979)
- 1.40 (shake flask-LSC, Veith et al. 1980)
- 2.67 (RP-HPLC-RT correlation, Veith et al. 1980)
- 2.21 (HPLC-RT correlation, McDuffie 1981)
- 2.70 (quoted from Veith et al. 1980, Veith & Kosian 1983; Davies & Dobbs 1984; Saito et al. 1992)
- 2.35 (20°C, shake flask-UV, Leyder & Boulanger 1983)
- 2.24, 2.29 (shake flask-HPLC/UV, HPLC-RT correlation, Howard et al. 1985)
- 2.47 (shake flask, unpublished data, Hansch & Leo 1985; 1987)
- 3.00 (RP-HPLC-RT correlation, De Koch & Lord 1987)
- 2.47 (recommended, Sangster 1993)
- 2.47 (recommended, Hansch et al. 1995)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 7.55 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

- 0.49–1.56 (calculated- K_{OW} , Veith et al. 1979, 1980)
- 2.07 (bluegill sunfish, Veith et al. 1980; Barrows et al. 1980; Veith & Kosian 1983)
- 1.86 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
- 1.08, 1.64 (calculated-S, calculated- K_{OW} , Lyman et al. 1982)
- 2.04 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 1.19 (mullet, Shimada et al. 1983)
- 2.10 (Davies & Dobbs 1984)
- 2.07 (fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 2.65 (calculated- K_{OW} , Wolfe et al. 1980a)
- 2.72 (soil, calculated-S, Lyman et al. 1982; quoted, Howard 1989)
- 1.97 (soil, calculated- K_{OW} , Lyman et al. 1982; quoted, Howard 1989)
- 2.15 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)

1.34	(sediment, calculated- K_{ow} , Pavlou & Weston 1983, 1984)
1.84	(Broome County of New York soil, shake flask-GC, Russell & McDuffie 1986)
3.00, 2.85, 3.24	(sediment, Alfisol soil, Podzol soil, von Oepen et al. 1991)
2.03	(activated carbon, calculated-MCI χ , Blum et al. 1994)
1.99	(calculated- K_{ow} , Kollig 1993)
1.84	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
1.84	(sediment/soil, selected, Staples et al. 1997)
4.90	(suspended solids, calculated- K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a)

Oxidation: rate constant k , for gas-phase second order rate constants, k_{OH} for reaction with OH radical, k_{NO_3} with NO_3 radical and k_{O_3} with O_3 or as indicated, *data at other temperatures see reference:

$k(aq.) = 18 \text{ M s}^{-1}$ in aquatic environment (Wolfe et al. 1980a)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1.4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

$k_{OH} = 1.08 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ corresponding to $t_{1/2} = 22.2 \text{ h}$ and the alkyl peroxy reaction $t_{1/2}(\text{calc}) = 6.5 \text{ yr}$ (Howard 1989)

photooxidation $t_{1/2} = 21\text{--}212 \text{ h}$ in air, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photooxidation $t_{1/2} = 2.4\text{--}12.2 \text{ yr}$ in water, based on estimated rate data for the reaction with alkyloxyl radical in aqueous solution (Howard et al. 1991)

$k(aq.) = (0.14 \pm 0.05) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with $t_{1/2} = 2.8 \text{ d}$ at pH 7 (Yao & Haag 1991).

$k_{OH}(aq.) = 4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ for the reaction with OH radical in aqueous solution (Haag & Yao 1992)

predicted atmospheric photooxidation $t_{1/2} = 1.8\text{--}18 \text{ d}$ from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)

$k_{OH} = 3.466 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 2.39 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis: $k(\text{acid-catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{alkaline}) = 79 \text{ M}^{-1} \text{ h}^{-1}$; phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4$ months to 100 yr at pH 8 and 30°C (Wolfe et al. 1980a)

$k(\text{second-order alkaline}) = 2.5 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C (Wolfe et al. 1980b; quoted, Kollig 1993)

$k(\text{alkaline}) = 2.5 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C and $k(\text{second-order alkaline rate}) = 1.2 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$ at pH 10–12 at 30°C , with a calculated $t_{1/2} = 18.3 \text{ yr}$ at pH 7 (Callahan et al. 1979)

First order hydrolysis $t_{1/2} = 8.8 \text{ yr}$ based on base rate constant at 30°C and pH 7; base rate constant $k = 90 \text{ M}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 32 \text{ d}$ based on measured rate constant at 30°C and pH from 10 to 12 (Howard et al. 1991)

$t_{1/2} = 3200 \text{ d}$, $t_{1/2} = 0.032 \text{ d}$ in natural waters (Capel & Larson 1995)

first-order hydrolysis $t_{1/2} = 8.8 \text{ yr}$ at pH 7 and $t_{1/2} = 32 \text{ d}$ at pH 10–12 based on base rate constant at 30°C (Howard et al. 1991; selected, Staples et al. 1997)

Biodegradation: microbial degradation $t_{1/2} = 10.5 \text{ d}$ by microorganisms isolated from soil and waste water at 30°C (Kurane et al. 1977, quoted, Russell et al. 1985);

estimated rate constant $k \sim (6.59 \pm 0.43) \times 10^2 \text{ min}^{-1}$ from retention times of reverse phase chromatography (Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985);

microbial degradation $k = 2 \times 10^{-4} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a);

0 to 32% mineralization in > 8 wk in municipal digested sludge (Horowitz et al. 1982);

complete degradation in 7.0 d for 5 and 10 ppm DEP in domestic waste water under aerobic conditions at 25°C (Tabak et al. 1981; quoted, Howard 1989);

$k = 0.315 \text{ d}^{-1}$ corresponding to $t_{1/2} = 2.21 \text{ d}$ with a mixed microbial population and underwent > 99% degradation in 28-d in shake flask biodegradation experiment (Sugatt et al. 1984);

greater than 90% of DEP was degraded within 40 d in digested sludge (Shelton et al. 1984); 85% biodegraded after 14 d incubation in aerobic freshwater sediments at 22°C (Johnson et al. 1984);

biodegraded in excess of 90% in less than 24 h in activated sludge systems (O'Grady et al. 1985);

soil-water biodegradation studies showed the 86% loss after 120 h in Broome County soils and 67% loss in leachate sprayed soil after 48 h (Russell et al. 1985);

anaerobic digestion of sludge with first-order $k = 6.0 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 115 \text{ h}$ (Ziogou et al. 1989)

aqueous aerobic $t_{1/2} = 72\text{--}1344 \text{ h}$, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991); aqueous anaerobic $t_{1/2} = 672\text{--}5376 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life and anaerobic screening test data (Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 3 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 28 \text{ d}$ in natural waters (Capel & Larson 1995)

Aerobic biodegradation in aquatic environments, first order $k = 1.8 \text{ d}^{-1}$ with $t_{1/2} = 0.39 \text{ d}$ in river water, $k = 0.16 \text{ d}^{-1}$ with $t_{1/2} = 4.33 \text{ d}$ in MITI inoculum, and $k = 0.98 \text{ d}^{-1}$ with $t_{1/2} = 0.71 \text{ d}$ (Peterson & Staples 2003)

biodegradation in aerobic soil, pseudo-first-order $k = 0.38 \text{ d}^{-1}$ with $t_{1/2} = 1.83 \text{ d}$ in agitated aqueous suspension.

For anaerobic degradation, first order rate $k = 0.069$ to $> 0.3 \text{ d}^{-1}$ with $t_{1/2} = 10.0$ to $< 2.3 \text{ d}$ in digester sludge, batch incubation; $k = 0.036 \text{ d}^{-1}$ with $t_{1/2} = 19.3 \text{ d}$ in flood soil; $k = 0.27 \text{ d}^{-1}$ with $t_{1/2} = 2.6 \text{ d}$ in pond sediment, $k = 0.13 \text{ d}^{-1}$ with $t_{1/2} = 5.3 \text{ d}$ in 10% freshwater sediment and $k = 0.31 \text{ d}^{-1}$ with $t_{1/2} = 2.2 \text{ d}$ in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: experimentally determined microbial $k = 3.2 \times 10^{-9} \text{ mL organism}^{-1} \text{ h}^{-1}$ (Wolfe et al. 1980a,c); estimated $k \sim 1 \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982);

mean microbial $k = (7.2 \pm 15.4) \times 10^{-7} \text{ mL cell}^{-1} \text{ h}^{-1}$ for 54 batch aufwuchs cultures (Lewis & Holm 1981; Lewis et al. 1984).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

depuration half-life $24 \text{ h} < t_{1/2} < 48 \text{ h}$ in tissues of bluegill sunfish (Barrows et al. 1980).

$k_2 = 6.83 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.584 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: an estimated $t_{1/2} = 22.2 \text{ h}$ for the vapor reaction with photochemically generated $8 \times 10^5 \text{ molecules}\cdot\text{cm}^{-3}$ OH radical in air at 25°C with an estimated $k \sim 1.08 \times 10^{-11} \text{ cm}^3\cdot\text{molecule}^{-1}\cdot\text{s}^{-1}$ (Howard 1989);

$t_{1/2} = 21\text{--}212 \text{ h}$, based on an estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photodegradation $t_{1/2} = 2.39 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 2.21 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984);

$t_{1/2} \sim 2 \text{ d}$ to $> 2 \text{ wk}$ for aerobic biodegradation in water; $t_{1/2} = 3 \text{ d}$ when incubated in dirty river water (Howard 1989);

overall degradation $t_{1/2} = 72\text{--}1344 \text{ h}$, based on aerobic aqueous grab sample data for fresh and marine water (Howard et al. 1991);

$k(\text{exptl}) = (0.14 \pm 0.5) \text{ M}^{-1} \text{ s}^{-1}$ for direct reaction with ozone in water at pH 2 and 22°C , with $t_{1/2} = 2.8 \text{ d}$ at pH 7 (Yao & Haag 1991).

Ground water: $t_{1/2} = 144\text{--}2688 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: $t_{1/2} < 14 \text{ d}$ in freshwater sediment (Johnson et al. 1984).

Soil: degradation $t_{1/2} = 10.5 \text{ d}$ by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977);

$t_{1/2} = 10\text{--}50 \text{ d}$ via volatilization subject to plant uptake from soil (Ryan et al. 1988);

$t_{1/2} = 72\text{--}1344 \text{ h}$, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota: $24 \text{ h} < t_{1/2} < 48 \text{ h}$ in tissues of bluegill sunfish (Barrows et al. 1980).

TABLE 15.1.3.2.1

Reported vapor pressures and aqueous solubilities of diethyl phthalate at various pressures and solubilities

Aqueous solubility				Vapor pressure			
Schwarz & Miller 1980		Thomsen et al. 2001		Stull 1947		Grayson & Fosbraey 1982	
elution chromatography-UV		shake flask-surface tension		summary of literature data		gas saturation-GC	
t/°C	g m ⁻³	t/°C	g m ⁻³	t/°C	P/Pa	t/°C	P/Pa
20	1200	10	1113	108.8	133.3	34.2	0.222
20	1240	25	838	140.7	666.6	40.0	0.470
20	1160	35	741	156.0	1333	44.8	0.784
30	1370			173.6	2666	50.7	1.368
30	1400			192.1	5333	60.5	3.320
30	1340			204.1	7999	20	0.046
				219.5	13332		
				243.0	26664	ln P = A – B/(T/K)	
				267.5	53329		P/Pa
				294.0	101325	A	32.5
						B	10436

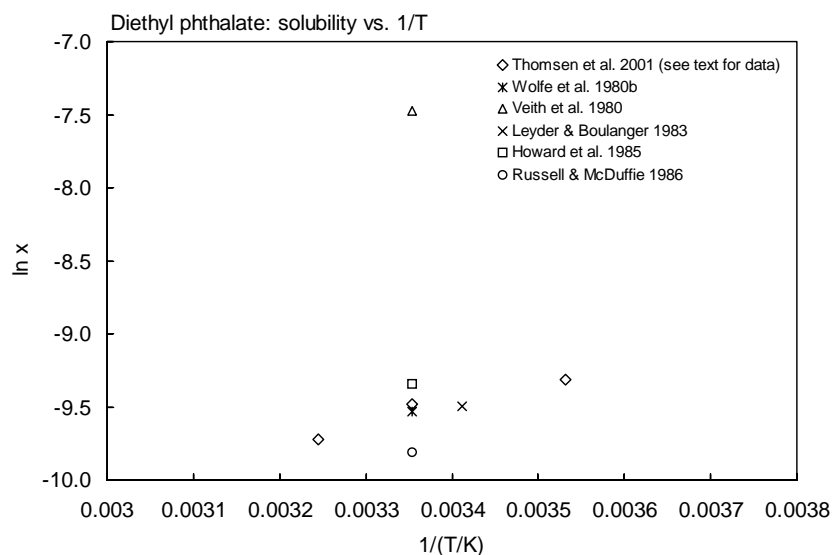


FIGURE 15.1.3.2.1 Logarithm of mole fraction solubility (ln x) versus reciprocal temperature for diethyl phthalate.

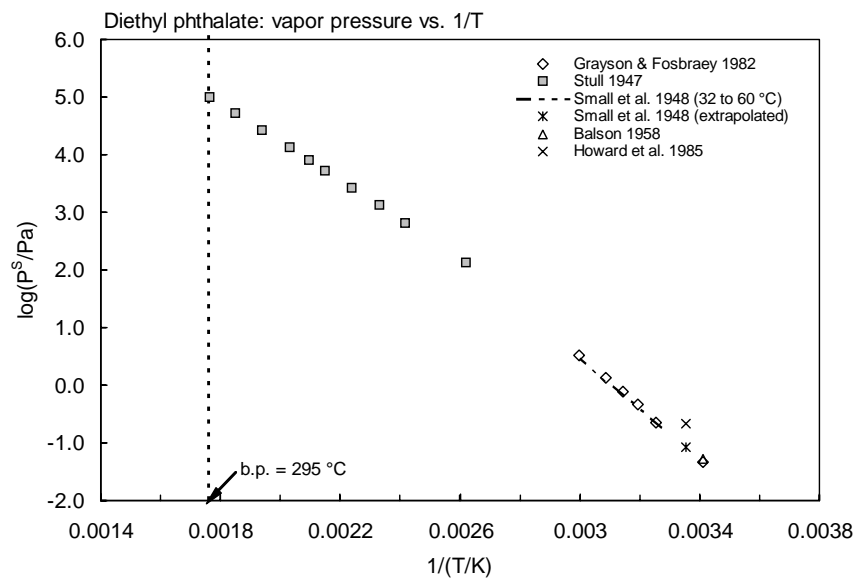
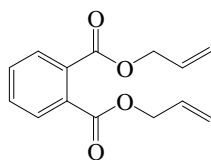


FIGURE 15.1.3.2.2 Logarithm of vapor pressure versus reciprocal temperature for diethyl phthalate.

15.1.3.3 Diallyl phthalate (DAP)



Common Name: Diallyl phthalate

Synonym: DAP

Chemical Name: di(2-propenyl) phthalate, bis(2-propenyl)ester, 1,2-benzenedicarboxylic acid

CAS Registry No: 131-17-9

Molecular Formula: $C_{14}H_{14}O_4$, $C_6H_4-1,2-(CO_2CH_2CH=CH_2)_2$

Molecular Weight: 246.259

Melting Point ($^{\circ}C$):

-77 (Fishbein & Albro 1972)

Boiling Point ($^{\circ}C$):

290 (Fishbein & Albro 1972)

Density (g/cm^3 at $20^{\circ}C$):

1.121 (Fishbein & Albro 1972)

Molar Volume (cm^3/mol):

219.7 ($20^{\circ}C$, calculated-density)

288.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

< 100 (Fishbein & Albro 1972)

182 ($20^{\circ}C$, shake flask-GC, Leyder & Boulanger 1983)

182; 43, 100 (recommended; calculated-QSAR, Staples 1997)

94 (calculated-UNIFAC, Thomsen et al. 1999)

156 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

0.0213; 0.00493, 0.155 (recommended; calculated-QSAR, Staples et al. 1997)

0.0271 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0289 (selected, Staples et al. 1997)

0.0428 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.23 (shake flask, Leyder & Boulanger 1983)

3.23 (recommended value, Sangster 1993)

3.23 (recommended, Hansch et al. 1995)

3.23; 3.37, 3.63 (recommended; calculated-QSAR, Staples 1997)

3.61 (calculated-UNIFAC, Thomsen et al. 1999)

3.11 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

7.87 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.04\text{--}0.4$ d (Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 2.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} = 0.04\text{--}0.4$ d (Staples et al. 1997).

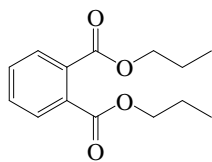
Surface water:

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 2.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

15.1.3.4 Di-*n*-propyl phthalate (DnPP)

Common Name: Di-*n*-propyl phthalate

Synonym: DPP, DNPP, dipropyl phthalate

Chemical Name: phthalic acid dipropyl ester; 1,2-benzenedicarboxylic acid dipropyl ester

CAS Registry No: 131-16-8

Molecular Formula: $C_{14}H_{18}O_4$, $C_6H_4[COOCH_2CH_2CH_3]_2$

Molecular Weight: 250.291

Melting Point ($^{\circ}C$):

-31.0 (Lide 2003)

Boiling Point ($^{\circ}C$):

304.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

232.2 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

302.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

88.70 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

108 (shake flask-UV, Leyder & Boulanger 1983)

108; 38, 47 (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)

77 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.0175 (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log(P/mmHg) = 11.66 - 4634/(T/K)$; temp range $32-75^{\circ}C$ or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, Small et al. 1948). Additional data at other temperatures designated * are compiled at the end of this section

$\log(P/kPa) = 8.625 - 3824/(T/K)$; temp range 403–578 K (Antoine eq., Stephenson & Malanowski 1987)

0.0119, 0.138 (calculated-QSAR, Staples et al. 1997)

0.0175 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0309 (recommended, Staples et al. 1997)

0.0569 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

3.27 (shake flask, Leyder & Boulanger 1983)

4.05 (HPLC-RT correlation, Hayward et al. 1990)

4.20 (HPLC-RT correlation, Jenke et al. 1990)

3.27, 4.05 (lit. values, Hansch et al. 1995)

3.27; 3.57, 3.63 (recommended; calculated-structure activity program, QSAR, Staples et al. 1997)

3.636 (Thomsen & Carlsen 1998)

3.40 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.04 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.9\text{--}9.0$ d (calculated, Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 6.5$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977);

rate constant $k = (10.71 \pm 0.73) \times 10^{-2} \text{ min}^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979).

Aerobic biodegradation in aquatic environments, first order $k = 1.3 \text{ d}^{-1}$ with $t_{1/2} = 0.53$ d in river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} = 0.9\text{--}9.0$ d (calculated, Staples et al. 1997).

Surface water: $t_{1/2} = 0.53$ d in river water (Peterson & Staples 2003)

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 6.5$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

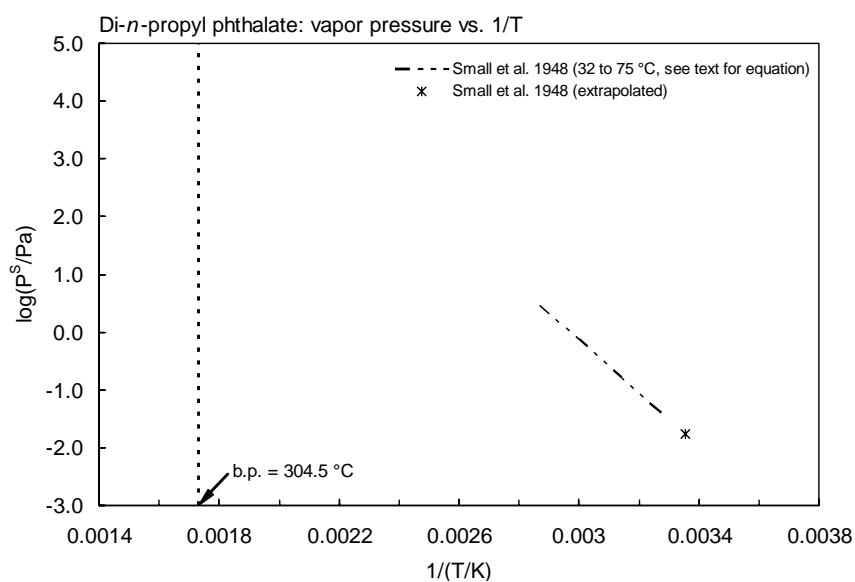
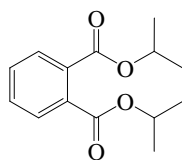


FIGURE 15.1.3.4.1 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-propyl phthalate.

15.1.3.5 Di-isopropyl phthalate (DIPP)



Common Name: Di-isopropyl phthalate

Synonym: DIPP

Chemical Name: phthalic acid dipropyl ester, bis(1-methylethyl)ester, 1,2-benzenedicarboxylic acid diisopropyl ester

CAS Registry No: 605-45-8

Molecular Formula: $C_{14}H_{18}O_4$, 1,2- $C_6H_4(CO_2C_3H_7)_2$

Molecular Weight: 250.291

Melting Point ($^{\circ}C$): liquid

Boiling Point ($^{\circ}C$):

304–305 (Weast 1982–83)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

302.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

322 (shake flask-UV, Leyder & Boulanger 1983)

136 (calculated-UNIFAC, Thomsen et al. 1999)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

2.83 (shake flask-UV, Leyder & Boulanger 1983)

2.83 (recommended, Sangster 1993)

2.83 (recommended, Hansch et al. 1995)

3.59 (calculated-UNIFAC, Thomsen et al. 1999)

Bioconcentration Factor, $\log BCF$:

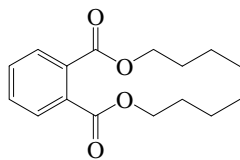
Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Biodegradation: degradation $t_{1/2} = 1.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at $30^{\circ}C$ (Kurane et al. 1977).

Half-Lives in the Environment:

Soil: degradation $t_{1/2} = 1.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at $30^{\circ}C$ (Kurane et al. 1977).

15.1.3.6 Di-*n*-butyl phthalate (DBP)

Common Name: Dibutyl phthalate

Synonym: *n*-butyl phthalate, di-*n*-butyl phthalate, DBP, dibutyl *o*-phthalate, *o*-benzenedicarboxylic acid dibutyl ester, benzene-*o*-dicarboxylic acid dibutyl ester

Chemical Name: phthalic acid dibutyl ester, di-*n*-butyl phthalate

CAS Registry No: 84-74-2

Molecular Formula: $C_{16}H_{22}O_4$, $o-C_6H_4(COOC_4H_9)_2$

Molecular Weight: 278.344

Melting Point ($^{\circ}C$):

-35.0 (Fishbein & Albro 1972; Verschueren 1977, 1983; Dean 1985; Howard 1989; Lide 2003)

Boiling Point ($^{\circ}C$):

340.0 (Stull 1947; Fishbein & Albro 1972; Weast 1982-83; Verschueren 1983; Dean 1985; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.0465 (21 $^{\circ}C$, Fishbein & Albro 1972)

1.047 (Weast 1982-83)

Molar Volume (cm^3/mol):

267.1 (calculated-density, Stephenson & Malanowski 1987)

347.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

93.3 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K) F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

11.08 (Deno & Berkheimer 1960)

4500 (Patty 1967)

4500 (Fishbein & Albro 1972)

10.0 (30 $^{\circ}C$, from Monsanto Chemical Co. data sheets, Peakall 1975)

13.0 (Wolfe et al. 1979; Wolfe et al. 1980a)

10.8, 11.1, 10.5 (20 $^{\circ}C$: quoted average, elution chromatography, UV, Schwarz & Miller 1980)

11.4, 11.5, 11.2 (30 $^{\circ}C$: quoted average, elution chromatography, UV, Schwarz & Miller 1980)

13 ± 1.6 , 4.45 (shake flask-GC, quoted, Wolfe et al. 1980b; quoted, Staples et al. 1997)

3.25 (solubility in 35 liter instant ocean, Giam et al. 1980)

10.1 (20 $^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

400, 4500 (Verschueren 1983)

28.0 (26 $^{\circ}C$, Verschueren 1983)

11.2 ± 0.3 (shake flask-HPLC/UV, Howard et al. 1985)

100 (Dean 1985)

11.2 (Howard et al. 1985)

9.40 (best estimate by turbidity inflection, DeFoe et al. 1990)

8.70, 9.40 (centrifugation-HPLC/UV, turbidity inflection-HPLC/UV, DeFoe et al. 1990)

11.2 (recommended, Staples et al. 1997)

9.90 (calculated-QSPR, Cousin & Mackay 2000)

13.3, 14.6, 5.50 (10, 25, 35 $^{\circ}C$, shake flask-surface tension measurement, Thomsen et al. 2001). Additional data at other temperatures designated * are compiled at the end of this section

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated *, are compiled at the end of this section):

- 13.33* (89°C, ebulliometry, measured range 89–176°C, Gardner & Brewer 1937)
 0.00233 (20°C, extrapolated, tensimeter, measured range 52–97°C, Hickman et al. 1937)
 $\log(P/\mu\text{mHg}) = 14.215 - 4680/(T/K)$; temp range 52–97°C (Hickman et al. 1937)
 0.0171* (20°C, extrapolated, effusion, measured range 40–95°C, Verhoek & Marshall 1939)
 $\log(P/\mu\text{mHg}) = 15.589 - 5122/(T/K)$; temp range 40–95°C (Verhoek & Marshall 1939)
 0.00253* (ebulliometry, extrapolated from graph, measured range 50–172°C, Burrows 1946)
 0.0217* (extrapolated-regression of tabulated data, temp range 148.2–340°C, Stull 1947)
 0.00345, 0.0043 (effusion method, extrapolated-Antoine eq., Small et al. 1948)
 $\log(P/\text{mmHg}) = 11.75 - 4871/(T/K)$; temp range ~ 32–75°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, Small et al. 1948)
 $\log(P/\text{mmHg}) = 11.86 - 4875/(T/K)$; temp range ~ 40–95°C or pressure range 5×10^{-2} to 10^{-4} mmHg (redistilled technical grade, Antoine eq., effusion method, Small et al. 1948)
 0.00276 (extrapolated-combined vapor pressure eq., Small et al. 1948)
 $\log(P/\text{mmHg}) = 7.065 - 1666/(T/K) - 547700/(T/K)^2$; temp range ~ 35–352°C (combined vapor pressure eq. derived from effusion measurement results and other published data, Small et al. 1948)
 0.0033 (20°C, extrapolated, tensimeter, measured range 55–102°C, Perry & Weber 1949)
 $\log(P/\mu\text{mHg}) = 13.58 - 4450/(T/K)$; temp range 55–102°C (pendulum-tensimeter method, Perry & Weber 1949)
 0.00364* (effusion method, measured range 19.9–44°C, Birks & Bradley 1949)
 7.6×10^{-5} (dew-point method and tensimeter method, temp range of 72–185°C, extrapolated-Antoine eq., Werner 1952)
 $\log(P/\mu\text{mHg}) = 11.008 - 2872/(176.5 + t/^{\circ}\text{C})$; temp range 72–185°C (Antoine eq., dew-point method and tensimeter method, Werner 1952)
 32* (125.7°C, vapor-liquid equilibrium data, measured range 125.7–202.5°C, Hammer & Lydersen 1957)
 $\log(P/\text{kPa}) = 6.439 - 1011/(T/K) - 720000/(T/K)^2$; temp range 125.7–202.5°C, Hammer & Lydersen 1957)
 1.53* (86.5°C, transpiration method, measured range 86.5–144°C, Franck 1969)
 $\log(P/\text{mmHg}) = [-0.2185 \times 17747.0/(T/K)] + 9.217428$; temp range: 148.2–340°C, (Antoine eq., Weast 1972–73)
 3.87×10^{-4} (6.55°C, submicron droplet evaporation, measured range 6.55–12.55°C, Ray et al. 1979)
 $\log(P/\text{mmHg}) = 12.217 - 4993/(T/K)$; temp range 6.55–12.55°C (submicron droplet evaporation, Ray et al. 1979)
 0.00206* (20°C, transpiration-GC “collection” measurement, Hales et al. 1981)
 $\ln(P/\text{Pa}) = 27.5178 - 8739.43/(T/K) - 330691/(T/K)^2$; temp range 293–373 K (empirical vapor pressure eq., from transpiration-GC measurement, Hales et al. 1981)
 0.0023* (20°C, vapor pressure balance, temp range 10–50°C, OECD 1981)
 0.00277 (20°C, evaporation rate-gravimetric method, Gückel et al. 1982)
 0.00133 (gas saturation, Jaber et al. 1982)
 0.40, 0.0653, 1.0 (structure-based estimation methods, Tucker et al. 1983)
 1.55×10^{-4} (extrapolated-Antoine eq., Boublik et al. 1984)
 $\log(P/\text{kPa}) = 576561 - 1744.128/(188.880 + t/^{\circ}\text{C})$, temp range 125.8–202.5°C (Antoine eq. derived from exptl. data of Hammer & Lydersen 1957, Boublik et al. 1984)
 0.00230 (OECD 1981 Guidelines, Dobbs et al. 1984)
 0.0011 (saturated column-HPLC/UV, Howard et al. 1985)
 0.00355 (extrapolated, Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 6.8788 - 2538.4/(-92.25 + T/K)$; temp range 314–469 K (Antoine eq.-I, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 7.97157 - 3385.9/(-37.18 + T/K)$; temp range 468–605 K (Antoine eq.-II, Stephenson & Malanowski 1987)
 0.0244 (calculated-solvatochromic parameters, Banerjee et al. 1990)
 0.0056 (GC-RT correlation, Hinckley et al. 1990)
 $\log(P/\text{mmHg}) = 6.63980 - 1744.20/(113.69 + t/^{\circ}\text{C})$, temp range 126–202°C (Antoine eq., 1992)
 $\log(P/\text{mmHg}) = 152.675 - 1.0754 \times 10^4/(T/K) - 51.17 \cdot \log(T/K) + 1.6933 \times 10^{-2} \cdot (T/K) + 2.4948 \times 10^{-14} \cdot (T/K)^2$; temp range 238–781 K (vapor pressure eq., Yaws et al. 1994)
 0.0027 (liquid P_L , GC-RT correlation, Donovan 1996)

- 0.0036 (recommended, Staples et al. 1997)
- 0.0473 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

- 0.1320 (calculated-P/C, Wolfe et al. 1980a)
- 0.0466 (Lyman et al. 1982; quoted, Howard 1989)
- 0.0284 (calculated-P/C, Mabey et al. 1982)
- 0.1835 (Atlas et al. 1983)
- 0.456, 0.446 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)
- 0.0297 (quoted from WERL Treatability Data, Ryan et al. 1988)
- 0.0895 (selected, Staples et al. 1997)
- 0.133 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

- 5.20 (calculated as per Leo et al. 1971, Callahan et al. 1979)
- 5.15 (RP-HPLC-RT correlation, Veith et al. 1979)
- 4.13 (HPLC-RT correlation; McDuffie 1981)
- 4.11, range 3.23–4.45 (shake flask-concn ratio, OECD 1981)
- 4.08 (shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
- 4.39, 4.56 (HPLC-extrapolated, Harnish et al. 1983)
- 4.57 (20°C , shake flask-UV, Leyder & Boulanger 1983)
- 4.79, 3.74 (shake flask-HPLC/UV, HPLC-RT, Howard et al. 1985)
- 4.11 (OECD value, Howard et al. 1985)
- 4.72 (shake flask, Hansch & Leo 1985; 1987)
- 4.57 (HPLC- k' correlation, Eadsforth 1986)
- 4.30 (HPLC-RT correlation, Haky & Leja 1986)
- 4.72 (measured value, DeFoe et al. 1990)
- 4.72 (recommended, Sangster 1993)
- 4.72 (recommended, Hansch et al. 1993)
- 4.01 (shake flask-dialysis tubing-HPLC/UV, both phases, Andersson & Schröder 1999)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

- 8.54 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log \text{BCF}$:

- 3.15 (fish, Mayer & Sanders 1973)
- 3.82, 3.70, 3.83, 3.28, 3.70, 3.43 (midge larvae, waterflea, scud, mayfly, grass shrimp, damselfly, Sanders et al. 1973)
- 3.83 (fish, Sanders et al. 1973)
- 1.32 (calculated, Kenaga 1980)
- 3.90 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
- 1.32–1.62, 0.46–1.49, 1.07 (oyster, shrimp, fish, Wofford et al. 1981)
- 1.50, 1.22, 1.07 (American oyster, brown shrimp, sheephead minnow, Wofford et al. 1981)
- 4.67 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
- 4.36 (*Selenastrum capricornutum*, Casserly et al. 1983)
- 1.32 (oyster, quoted from Wofford et al. 1981, Zaroogian et al. 1985)
- 3.68, 3.68 (oyster, estimated values, Zaroogian et al. 1985)
- 1.08 (fish, highest BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

- 2.20 (soil, estimated-S, Kenaga 1980)
- 3.81 (soil, estimated-S, Wolfe et al. 1980a)
- 2.17 (marine sediment/seawater with 1% organic carbon, Bouwer et al. 1981)
- 1.60, 1.30, 0.602 (between montmorillonite, kaolinite, calcium montmorillonite and seawater at concn. of 3–4 ppm, Sullivan et al. 1981)

- 0.301, 0.602, 1.556 (between montmorillonite, kaolinite, calcium montmorillonite and seawater at concn. of 20 ppb, Sullivan et al. 1981)
- 5.23 (sediment-water, calculated- K_{OW} , Mabey et al. 1982).
- 4.17 (sediment/soil, Sullivan et al. 1982; selected, Staples et al. 1997)
- 4.54 (sediment, calculated- K_{OW} , Pavlou & Weston 1983,84)
- 3.14 (Broome County soil in New York, shake flask-GC, Russell & McDuffie 1986)
- 4.37 (calculated- K_{OW} , Kollig 1993)
- 3.14 (quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
- 3.09, 5.20 (suspended solids, calculated- K_d assuming a 0.10 organic carbon fraction, Staples et al. 1997)
- 3.14; 3.76, 2.46, 2.86, 3.09, 3.12, 3.11 (quoted lit.; values obtained from HPLC- k' correlation on different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

- Volatilization: $t_{1/2} = 28$ d from a stirred seawater solution 1.0 m deep (Atlas et al. 1982; quoted, Howard 1989)
 evaporation rate $k = 3.42 \times 10^{-10}$ mol cm^{-2} h^{-1} at 20°C (Gückel et al. 1982);
 $t_{1/2} \sim 47$ d in a river of 1.0 m deep with 1 m/s current and a 3 m/s wind using Henry's law constant while the rate of volatilization being controlled by the diffusion through air (Lyman et al. 1982; quoted, Howard 1989).
- Photolysis: direct photolysis (near surface) rate constant $k \sim 2 \times 10^{-4}$ h^{-1} in natural water (Wolfe et al. 1980a)
 aqueous photolysis rate $k = 0.23$ h^{-1} and $t_{1/2} = 3$ h (Jin et al. 1999, quoted, Peterson & Staples 2003)
 Indirect photolysis $k = 0.29$ d^{-1} with $t_{1/2} = 2.4$ d in air (Peterson & Staples 2003).
- Oxidation:
 $k = 18$ M s^{-1} , the free radical oxidation rate constant (EXAMS model, Wolfe et al. 1980a)
 photooxidation $t_{1/2} = 2.4$ –12.2 yr in water, based on estimated rate data for the reaction with alkyloxyl radical in aqueous solution (Wolfe et al. 1980a; quoted, Howard et al. 1991)
 $k \ll 360$ M^{-1} h^{-1} for singlet oxygen and $k = 1.4$ M^{-1} h^{-1} for peroxy radical (Mabey et al. 1982)
 photooxidation $t_{1/2} = 18.4$ h with reaction with OH radical (Howard 1989)
 photooxidation $t_{1/2} = 7.4$ –74 h in air, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)
 Atmospheric photooxidation $t_{1/2} = 0.6$ –6.0 d from Atkinson 1988 atmospheric-oxidation program (estimated, Staples et al. 1997).
 $k_{OH} = 9.277 \times 10^{-12}$ cm^3 molecule $^{-1}$ s^{-1} and $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm^{-3} in air (Peterson & Staples 2003)

Hydrolysis:

- $k(\text{second-order alkaline}) = 2.2 \times 10^{-2}$ M^{-1} s^{-1} for pH 10–12 at 30°C, with calculated half-life of 10 yr at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979)
- $k(\text{acid catalyzed}) = 0.04$ M^{-1} h^{-1} , $k(\text{second order alkaline}) = 38$ M^{-1} h^{-1} in an aquatic environment (Wolfe et al. 1980a)
- $k(\text{second-order alkaline}) = (1.0 \pm 0.05) \times 10^{-2}$ M^{-1} s^{-1} at pH 7 and 30°C, with first-order hydrolysis $t_{1/2} = 10$ yr (Wolfe et al. 1980b; quoted, Kollig 1993);
- $t_{1/2} = 76$ d at pH 9 and $t_{1/2} = 10$ yr at neutral pH (estimated, Howard 1989)
- $t_{1/2} = 10$ yr, based on the overall hydrolysis rate constant (Howard et al. 1991)
- aqueous abiotic $t_{1/2} = 22$ yr (selected, Staples et al. 1997)
- $t_{1/2} = 3700$ d at pH 7, $t_{1/2} = 76$ d at pH 12 in natural waters (Capel & Larson 1995)

Biodegradation:

- $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)
- DBP was rapidly degraded, 3% left after 5 d, but under anaerobic conditions required 30 d for the degradation freshwater hydrosol, under aerobic conditions (Johnson et al. 1979, quoted, Russell et al. 1985)
- a 90% loss in 3 d from river water (Brinkman et al. 1979, quoted, Russell et al. 1985)
- $k = (13.26 \pm 0.73) \times 10^2$ min^{-1} (reversed phase-GC-RT correlation, Urushigawa & Yonezawa 1979; quoted, O'Grady et al. 1985)
- $k = 2.9 \times 10^{-8}$ mL organism^{-1} h^{-1} (Wolfe et al. 1980a);
- $k > 0.5$ d^{-1} , significant degradation with rapid adaptation within 7 d in an aerobic environment (Tabak et al. 1981; quoted, Mills et al. 1982);
- $k = 7.4 \times 10^{-7}$ mL cell^{-1} d^{-1} (river die-away test, Scow 1982);

32–85% degraded after 2–3 wk in municipal digested sludge (Horowitz et al. 1982)
decomposed within 80 d under both aerobic and anaerobic conditions when approximately 90% added to soils (Inman et al. 1984)

$k = (0.1\text{--}7.6) \times 10^{-4} \text{ h}^{-1}$ to $(4.9\text{--}36.5) \times 10^{-4} \text{ h}^{-1}$ for water and water/sediment systems (under sterile conditions); and $k = (29.3\text{--}409) \times 10^{-4} \text{ h}^{-1}$ to $(38.2\text{--}456) \times 10^{-4} \text{ h}^{-1}$ for water and water/sediment systems (under active conditions) samples from six estuarine and freshwater sites, actual $t_{1/2} = 1.0\text{--}4.8 \text{ d}$ for active sediment treatment, $t_{1/2} = 1.7\text{--}13.0 \text{ d}$ for active water treatment and $t_{1/2} = 8\text{--}23 \text{ d}$ for sterile sediment (Walker et al. 1984)

$k = 0.050 \text{ d}^{-1}$ and a $t_{1/2} = 15.4 \text{ d}$ in a shake flask biodegradation experiment (Sugatt et al. 1984)

> 90% of DBP was degraded within 40 d in digested sludge (Shelton et al. 1984)

> 90% biodegraded in less than 24 h in activated sludge systems (O'Grady et al. 1985)

81% loss in Broome County soils after 24 h and 70% loss in leachate sprayed soil after 24 h in soil-water biodegradation studies (Russell et al. 1985);

$k = 10.6 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 65 \text{ h}$, anaerobic digestion of sludge (Ziogou et al. 1989);

$t_{1/2} < 5 \text{ d}$, aerobic conditions, $t_{1/2} = 20 \text{ d}$ under anaerobic conditions in a garden soil (Shanker et al. 1985)

$t_{1/2} = 24\text{--}552 \text{ h}$, aqueous aerobic based on unacclimated aerobic river die-away test and soil grab sample data (Howard et al. 1991);

$t_{1/2} = 48\text{--}552 \text{ h}$, aqueous anaerobic, based on unacclimated anaerobic grab sample data for soil and sediment (Johnson & Lulves 1975; Verschueren 1983; Howard et al. 1991)

$t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2 \text{ d}$ in natural waters (Capel & Larson 1995)

$k = 0.0216 \text{ h}^{-1}$ with $t_{1/2} = 32.1 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000)

aerobic biodegradation in aquatic environments, first order $k = 0.8 \text{ d}^{-1}$ with $t_{1/2} = 0.87 \text{ d}$ in river water, $k = 0.51 \text{ d}^{-1}$ with $t_{1/2} = 1.56 \text{ d}$ in estuarine and river water, $k = 0.29 \text{ d}^{-1}$ with $t_{1/2} = 2.40 \text{ d}$ in sediment microcosm, $k = 0.22 \text{ d}^{-1}$ with $t_{1/2} = 3.15 \text{ d}$ in MITI inoculum, $k = 0.14 \text{ d}^{-1}$ with $t_{1/2} = 4.95 \text{ d}$ in river water, low sediment, and $k = 0.98 \text{ d}^{-1}$ with $t_{1/2} = 0.71 \text{ d}$ river water only (Peterson & Staples 2003)

biodegradation in aerobic soil, pseudo-first-order $k = 1.61 \text{ d}^{-1}$ with $t_{1/2} = 0.43 \text{ d}$ in agitated aqueous suspension, $k = 0.39 \text{ d}^{-1}$ with $t_{1/2} = 1.8 \text{ d}$ at 30°C garden soil; $k = 0.103 \text{ d}^{-1}$ with $t_{1/2} = 6.7 \text{ d}$ in soil with 2% OC; $k = 0.044 \text{ d}^{-1}$ with $t_{1/2} = 11.2 \text{ d}$ in soil with 3.3% OC and $k = 0.62 \text{ d}^{-1}$ with $t_{1/2} = 15.8 \text{ d}$ in soil with 1.6% OC. For anaerobic degradation, first order rate $k = 0.26\text{--}0.581 \text{ d}^{-1}$ with $t_{1/2} = 1.19\text{--}2.7 \text{ d}$ in undiluted digester sludge, $k = 0.025\text{--}0.073 \text{ d}^{-1}$ with $t_{1/2} = 27.7\text{--}9.5 \text{ d}$ in 10% diluted sludge, batch incubation; $k = 0.076 \text{ d}^{-1}$ with $t_{1/2} = 9 \text{ d}$ in 10% freshwater sediment and $k = 0.051 \text{ d}^{-1}$ with $t_{1/2} = 13 \text{ d}$ in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: $k = (1.9\text{--}4.4) \times 10^{-8} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Steen et al. 1979; quoted, Mabey et al. 1982; Steen 1991);

$k = 2.9 \times 10^{-8} \text{ mL cell}^{-1} \text{ h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or half-Lives:

$t_{1/2} = 3 \text{ d}$ in *Daphnia magna* (Mayer & Sanders 1973).

$k_2 = 0.237 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.0114 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} \sim 18 \text{ h}$ for the vapor phase reaction with hydroxyl radicals in air (Howard 1989);

$t_{1/2} = 7.4\text{--}74 \text{ h}$, based on estimated rate data for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

Photodegradation $t_{1/2} = 0.89 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air and indirect photolysis $t_{1/2} = 2.4 \text{ d}$ (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 15.4 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984)

$t_{1/2} = 2\text{--}12 \text{ d}$ in water alone (Howard 1989);

$t_{1/2} = 24\text{--}336 \text{ h}$, based on unacclimated aerobic river die-away test and fresh water/sediment grab sample data (Howard et al. 1991)

Biodegradation $t_{1/2}(\text{aerobic}) = 1 \text{ d}$, $t_{1/2}(\text{anaerobic}) = 2 \text{ d}$; hydrolysis $t_{1/2} = 3700 \text{ d}$ at pH 7 and $t_{1/2} = 76 \text{ d}$ at pH 12 in natural waters (Capel & Larson 1995)

biodegradation $t_{1/2} = 0.87\text{--}5.78 \text{ d}$ in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 48\text{--}552$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Sediment: 97% degradation in 5 d in an aerobic pond water-sediment mixture; $t_{1/2} = 7\text{--}30$ d under anaerobic conditions, $t_{1/2} = 1\text{--}5$ d in sediment-water systems of estuarine and freshwater sites (Howard 1989).

Soil: degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977) degradation $t_{1/2} = 11$ to 53 d as affected by soil type, pH, temperature, aeration status and sterilization (Inman et al. 1984);

biodegradation $t_{1/2}(\text{aerobic}) < 5$ d and $t_{1/2}(\text{anaerobic}) \sim 20$ d in a garden soil (Shanker et al. 1985);

$t_{1/2} = 10\text{--}50$ d via volatilization subject to plant uptake from soil (Ryan et al. 1988);

overall $t_{1/2} = 48\text{--}552$ h, based on unacclimated aerobic soil grab sample data (Howard et al. 1991)

Aerobic biodegradation in soil, $t_{1/2}$ ranging from 0.43 to 19.8 d in aqueous suspension, garden soil and soils with different organic carbon contents (Peterson & Staples 2003)

Biota: elimination $t_{1/2} = 3$ d for waterfleas *Daphnia magna* (Mayer & Sanders 1973).

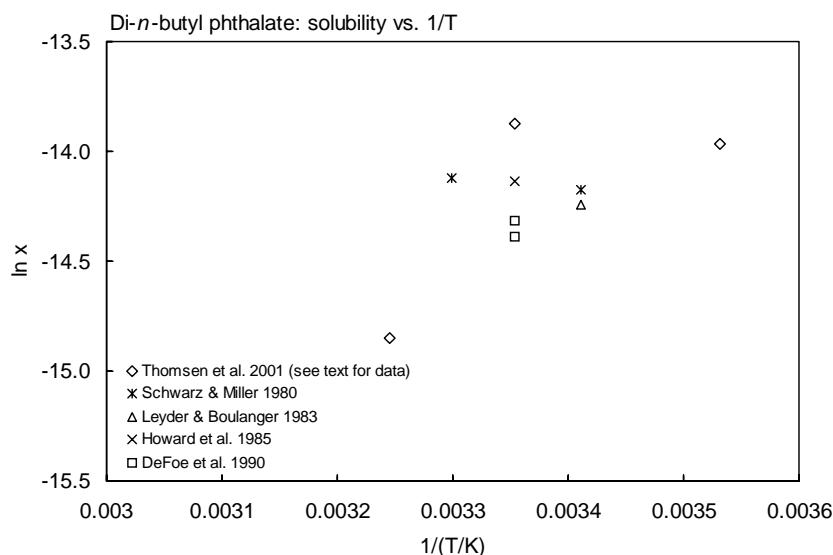


FIGURE 15.1.3.6.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for di-*n*-butyl phthalate.

TABLE 15.1.3.6.1

Reported vapor pressures of di-*n*-butyl phthalate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$	(1)	$\ln P = A - B/(T/K)$	(1a)
$\log P = A - B/(C + t/^\circ\text{C})$	(2)	$\ln P = A - B/(C + t/^\circ\text{C})$	(2a)
$\log P = A - B/(C + T/K)$	(3)		
$\log P = A - B/(T/K) - C \cdot \log(T/K)$	(4)		
$\log P = A - B/(T/K) - C/(T/K)^2$	(5)	$\ln P = A - B/(T/K) - C/(T/K)^2$	(5a)

1.

Gardner & Brewer 1937		Verhoek & Marshall 1939		Burrows 1946		Stull 1947	
ebulliometry		static and dynamic methods		ebulliometry		summary of literature data	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
89.0	13.33	40	0.0223	50	0.0667	148.2	133.3
98.8	53.33	55	0.137	82	1.333	182.1	666.6
106.1	79.99	55	0.109	120	26.66	198.2	1333

TABLE 15.1.3.6.1 (Continued)

Gardner & Brewer 1937		Verhoek & Marshall 1939		Burrows 1946		Stull 1947	
ebulliometry		static and dynamic methods		ebulliometry		summary of literature data	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
111.3	106.7	59.7	0.237	147	133.3	216.2	2666
122.5	120.0	64.7	0.393	172	533.3	235.8	5333
132.0	133.3	65.0	0.409	25	0.00253*	247.8	7999
134.5	120.0	69.7	0.612		*extrapolated	263.7	13332
137.2	133.32	70.0	0.601			287.0	26664
138.0	133.32	74.6	0.981			313.5	53329
141.0	146.7	75.0	1.076			340.0	101325
141.2	146.7	75.0	0.904				
144.8	160.0	85.0	2.880			mp/°C	—
145.4	146.7	85.0	2.520				
147.5	173.3	85.0	2.520				
148.0	160.0	95.0	6.040				
149.5	173.3						
150.0	186.7						
151.0	173.3	eq. 1	P/microns				
153.5	200.0	A	15.589				
162.9	280.0	B	5122				
164.4	293.3						
167.2	373.3	$\Delta H_v = 98.07$ kJ/mol					
168.0	373.3						
168.6	386.6						
171.8	426.6						
176.3	546.6						
bp/°C	340.7						

2.

Small et al. 1948		Birks & Bradley 1949		Hammer & Lydersen 1957		Franck 1969	
effusion		effusion		vapor-liquid equilibrium		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
exptl data presented in graph		19.9	0.001907	125.7	32.0	86.5	1.53
		23.0	0.002733	131.55	49.06	86.5	1.63
eq. 2	P/mmHg	25.0	0.003640	139.21	73.86	86.5	1.76
A	11.75	30.0	0.006666	147.02	120	105.5	9.42
B	4871	35	0.01180	156.70	205	105.6	9.88
measured pressure range:		40	0.02106	158.89	228	105.5	10.5
0.05 to 0.001 mmHg		43	0.02933	162.12	277	125.5	37.8
$\Delta H_v = 93.30$ kJ/mol		43.5	0.02959	172.76	480	125.5	36.9
		44	0.03346	180.18	671	125.5	34.9
for redistilled tech. grade				180.36	667	144.5	136.0
eq. 2	P/mmHg	eq. 2	P/mmHg	186.87	921	144.5	109.0
A	11.86	A		195.88	1353	144.5	103.0
B	4875	B		202.05	1739		
$\Delta H_v = 93.30$ kJ/mol		C					

(Continued)

TABLE 15.1.3.6.1 (Continued)

Small et al. 1947		Birks & Bradley 1949		Hammer & Lydersen 1957		Franck 1969	
effusion		effusion		vapor-liquid equilibrium		transpiration method	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
Werner 1952 dew-point/tensimeter method t/°C P/Pa				eq. 5	P/kPa	OECD 1981	
				A	6.439	vapor pressure balance	
				B	1011	t/°C	P/Pa
				C	720000	10	6.5×10^{-4}
exptl data presented in graph eq. 2 P/mmHg A 11.008 B 2872 C 176.5				In Boublik et al. 1984		20	2.3×10^{-3}
				A	5.76561	30	7.8×10^{-3}
				B	1744.128	40	2.4×10^{-2}
				C	113.731	50	7.0×10^{-2}
				bp/°C	188.880		
temp range: 70–170°C							

3.

Hales et al. 1981

transpiration-GC analysis							
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
collection		continued		continued		overall best fit equation:	
39.89	0.02398	80.02	1.162	19.90	2.064×10^{-3}	eq. 5a	P/Pa
39.92	0.02333	79.95	1.089	20.0	2.065×10^{-3}	A	21.5178
39.92	0.02273	99.93	5.335	30.1	7.252×10^{-3}	B	8739.43
39.92	0.02321	100.2	5.648	30.15	7.428×10^{-3}	C	330691
60.18	0.1917	99.94	5.833	40.7	0.02461		
60.03	0.1734	for small saturator		60.01	0.1826		
60.06	0.1858	19.85	0.002224	79.96	1.130		
60.06	0.1779	19.90	0.002160	79.92	1.112		
60.16	0.1842	30.11	0.007276	100.09	5.798		
79.98	1.104	30.13	0.007481				
79.96	1.099	60.27	0.1996				

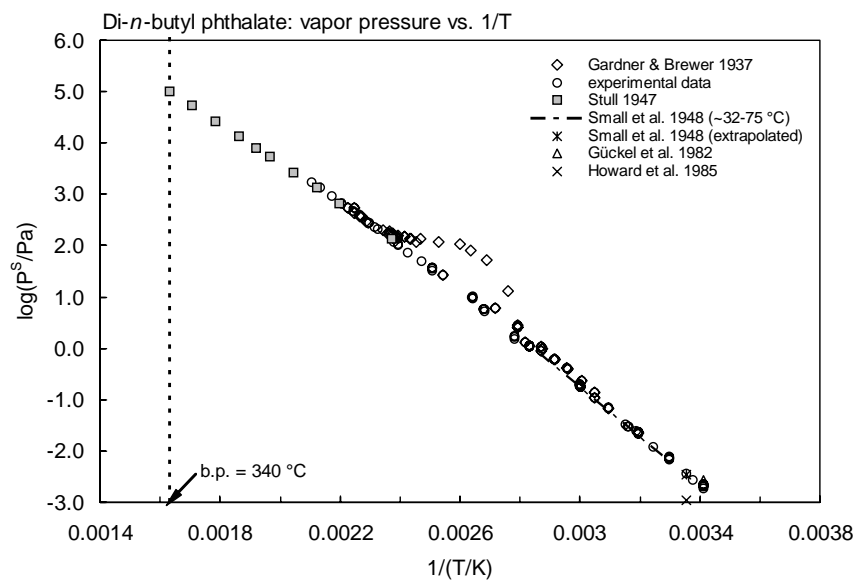
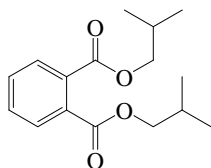


FIGURE 15.1.3.6.2 Logarithm of vapor pressure versus reciprocal temperature for di-*n*-butyl phthalate.

15.1.3.7 Di-isobutyl phthalate (DIBP)



Common Name: Di-isobutyl phthalate

Synonym: DIBP

Chemical Name: phthalic acid diisobutyl ester, bis(2-methylpropyl)ester, 1,2-benzenedicarboxylic acid

CAS Registry No: 84-69-5

Molecular Formula: $C_{16}H_{22}O_4$

Molecular Weight: 278.344

Melting Point ($^{\circ}C$):

-58 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

296.5 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.040 (Fishbein & Albro 1972)

1.049 ($15^{\circ}C$, Weast 1982-83)

Molar Volume (cm^3/mol):

347.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

100 (Fishbein & Albro 1972)

6.20 (shake flask-nephelometry, Hollifield 1979)

20.3 (Leyder & Boulanger 1983)

20.0; 5.1, 9.6 (recommended; calculated-QSAR, Staples et al. 1997)

21.6 (calculated-UNIFAC, Thomsen et al. 1999)

9.90 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

2.4×10^{-4} , 0.0773 (calculated-QSAR, Staples et al. 1997)

0.00473 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa m^3/mol$ at $25^{\circ}C$):

0.0185 (recommended, Staples et al. 1997)

0.133 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.11 (shake flask, Leyder & Boulanger 1983)

4.43 (calculated-QSAR, Matthiessen et al. 1992)

4.11 (quoted and recommended, Sangster 1993)

4.11 (recommended, Hansch et al. 1995)

4.11; 4.31, 4.46 (recommended; calculated-QSAR, Staples et al. 1997)

4.46 (calculated-UNIFAC, Thomsen et al. 1999)

4.27 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

3.10 (calculated-QSAR, fish, Matthiessen et al. 1992)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.14 (calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
3.01 (suspended solids, Staples et al. 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.6\text{--}6.0$ d (calculated, Staples et al. 1997)

$k_{OH} = 9.280 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003).

Hydrolysis:

$k(\text{second-order alkaline}) = (1.4 - 0.2) \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C in water (Wolfe et al. 1980b)

Biodegradation: degradation $t_{1/2} = 3.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Aerobic biodegradation in aquatic environments, first order $k = 0.8 \text{ d}^{-1}$ with $t_{1/2} = 0.87$ d in river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_2 = 0.134 \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.0114 \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: atmospheric photooxidation half-life of $0.6\text{--}6.0$ d (calculated, Staples et al. 1997).

photodegradation $t_{1/2} = 0.89$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} = 0.87$ d in river water (Peterson & Staples 2003)

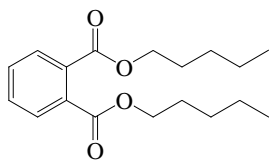
Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 3.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

15.1.3.8 Dipentyl phthalate (DPP)



Common Name: Dipentyl phthalate

Synonym: DPpP, di-*n*-amyl phthalate

Chemical Name: dipentyl phthalate, phthalic acid diphenyl ester, 1,2-benzenedicarboxylic acid diphenyl ester

CAS Registry No: 131-18-0

Molecular Formula: C₁₈H₂₆O₄

Molecular Weight: 306.397

Melting Point (°C):

< -54.5 (Stephenson & Malanowski 1987)

Boiling Point (°C):

342 (Stephenson & Malanowski 1987)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

299.8 (16°C, Stephenson & Malanowski 1987)

391.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

99.16 (Small et al. 1948)

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

0.082 (shake flask-nephelometry, Hollifield 1979)

0.1–0.8 (shake flask-GC, Leyder & Boulanger 1983)

0.522, 1.69 (quoted, calculated-UNIFAC, Thomsen et al. 1999)

1.30 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at 25°C and reported temperature dependence equations):

5.68×10^{-4} (effusion method, extrapolated-Antoine eq., Small et al. 1948)

$\log(P/\text{mmHg}) = 12.04 - 5191/(T/K)$; temp range 55–102°C or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion, data presented in graph, Small et al. 1948) (See figure at the end of this section.)

0.0014 (20°C, extrapolated, tensimeter, measured range 63–111°C, Perry & Weber 1949)

$\log(P/\mu\text{mHg}) = 13.57 - 4560/(T/K)$; temp range 63–111°C (pendulum-tensimeter method, Perry & Weber 1949)

5.68×10^{-4} (extrapolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/\text{kPa}) = 11.165 - 5191/(T/K)$; temp range 303–500 K (Antoine eq., liquid, Stephenson & Malanowski 1987)

0.00128 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.302 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{ow}:

4.85 (shake flask, Leyder & Boulanger 1983; quoted, Sangster 1993, Hansch et al. 1995)

5.33 (calculated-UNIFAC, Thomsen et al. 1999)

5.12, 5.62 (calculated-QSPR, quoted lit., Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.03 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 9.0$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977);

rate constant $k = (9.12 \pm 1.51) \times 10^{-2} \text{ min}^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979).

aerobic biodegradation in aquatic environments, first order $k = 1.3 \text{ d}^{-1}$ with $t_{1/2} = 5.3$ d in river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: biodegradation $t_{1/2} = 5.3$ d in aerobic aquatic environments (Peterson & Staples 2003)

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 9.0$ d by microorganisms (*Pseudomonas acidovorans* 256-1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

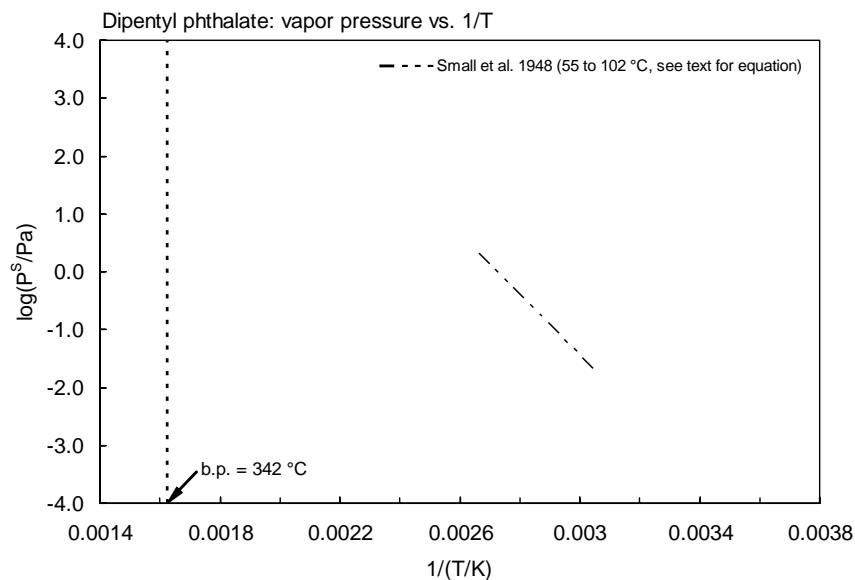
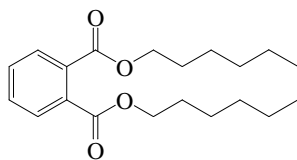


FIGURE 15.1.3.8.1 Logarithm of vapor pressure versus reciprocal temperature for dipentyl phthalate.

15.1.3.9 Di-*n*-hexyl phthalate (DHP)

Common Name: Di-*n*-hexyl phthalate

Synonym: DHP, DnH(6)P

Chemical Name: Di-*n*-hexyl phthalate, dihexyl ester, 1,2-benzenedicarboxylic acid

CAS Registry No: 84-75-3, 68515-50-4

Molecular Formula: $C_{20}H_{30}O_4$, $C_6H_4[COOCH_2(CH_2)_4CH_3]_2$

Molecular Weight: 334.450

Melting Point ($^{\circ}C$):

-27.4 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.990 (Fishbein & Abro 1972)

Molar Volume (cm^3/mol):

227.8 ($20^{\circ}C$, calculated-density)

436.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

102.9 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

insoluble (Fishbein & Abro 1972)

0.24 (shake flask-HPLC/UV, Howard et al. 1985)

0.05; 0.19, 0.049 (recommended; calculated-QSAR, Staples et al. 1997)

0.046 (shake flask-GC, Ellington 1999)

0.47 (calculated-UNIFAC method, Thomsen et al. 1999)

0.159 (calculated-QSPR, Cousins & Mackay 2000)

0.94, 0.52, 0.38 (10, 25, $35^{\circ}C$, shake flask-surface tension measurement, Thomsen et al. 2001) (See figure at the end of this section.)

0.070 ($20^{\circ}C$, shake flask-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

$\log(P/mmHg) = 11.98 - 5381/(T/K)$; temp range 72 – $112^{\circ}C$ or pressure range 5×10^{-2} to 10^{-4} mmHg (Antoine eq., effusion method, data presented in graph, Small et al. 1948) (See figure at the end of this section.)

667 (at $210^{\circ}C$, Fishbein & Abro 1972)

1.03×10^{-3} (Antoine eq., interpolated-Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = -1.01167 - 1483.636/(T/K)$; temp range 288 – 303 K (Antoine eq.-I, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 11.105 - 5382/(T/K)$; temp range 343 – 387 K (Antoine eq.-II, liquid, Stephenson & Malanowski 1987)

$\log(P_L/kPa) = -9.785 - 4805/(T/K)$; temp range 453 – 533 K (Antoine eq.-III for liquid, Stephenson & Malanowski 1987)

1.90×10^{-3} (gas saturation-GC, Howard et al. 1985)

0.267 (quoted, Giam et al. 1994)

0.67; 2.53×10^{-6} , 1.6×10^{-3} (recommended; calculated-QSAR, Staples et al. 1997)

0.000345 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$ at 25°C):

4.46	(recommended, Staples et al. 1997)
0.726	(calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{\text{OW}}$:

5.65–5.91	(HPLC-RT correlation, Howard et al. 1985)
5.80	(quoted value of Howard et al. 1985, Sangster 1993)
5.80	(Hansch et al. 1995)
6.30; 6.57, 6.67	(recommended; calculated-QSAR, Staples et al. 1997)
6.20	(calculated-UNFAC, Thomsen et al. 1999)
6.00	(calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{\text{OA}}$:

9.53	(calculated-QSPR, Cousins & Mackay 2000)
------	--

Bioconcentration Factor, $\log \text{BCF}$:

Sorption Partition Coefficient, $\log K_{\text{OC}}$:

4.72	(soil/sediment, Staples et al. 1997)
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Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0$ d (calculated, Staples et al. 1997).

$k_{\text{OH}} = 14.929 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.55$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: rate constant $k = (6.86 \pm 0.23) \times 10^{-2} \text{ min}^{-1}$ was estimated from the retention time in reverse phase chromatography (Urushigawa & Yonezawa 1979);
primary biodegradation rate constant $k = 0.241 \text{ d}^{-1}$ and $t_{1/2} = 2.93$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0$ d (calculated, Staples et al. 1997).

Photodegradation $t_{1/2} = 0.55$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: primary biodegradation rate constant $k = 0.241 \text{ d}^{-1}$ and $t_{1/2} = 2.93$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

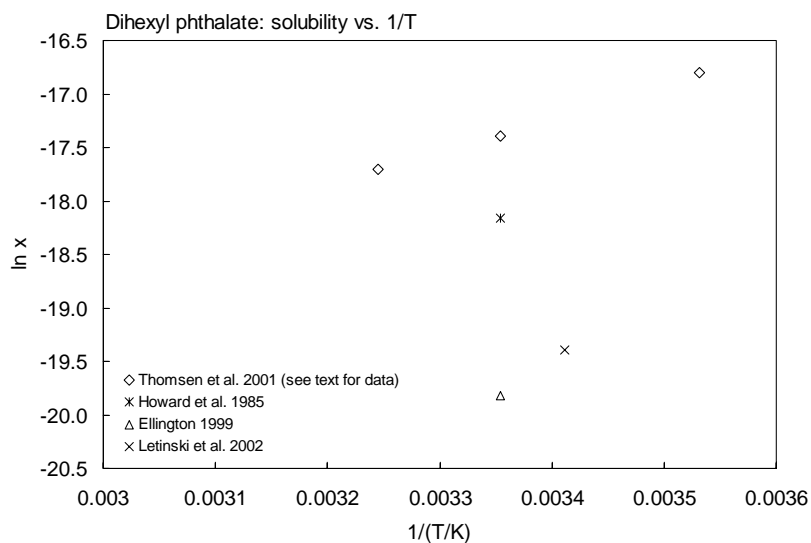


FIGURE 15.1.3.9.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for dihexyl phthalate.

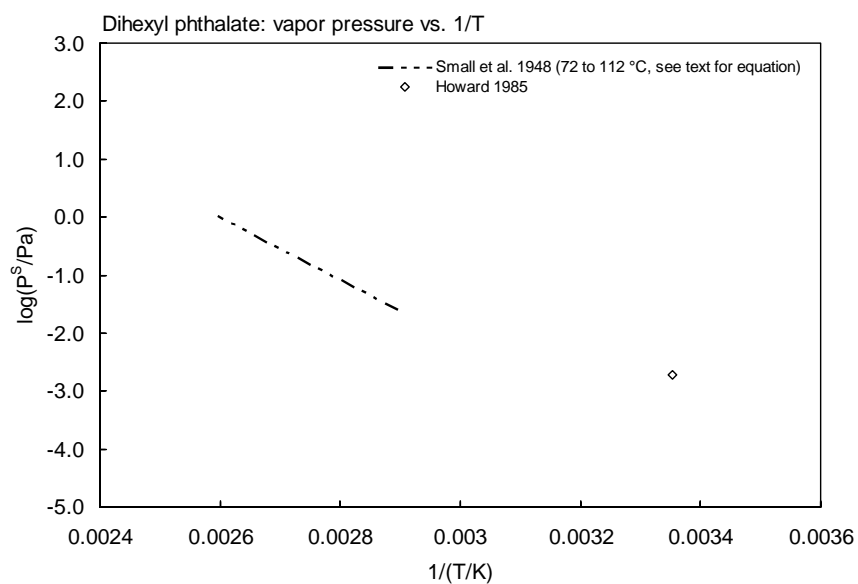
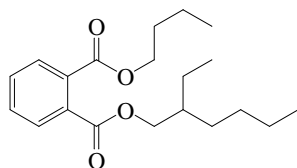


FIGURE 15.1.3.9.2 Logarithm of vapor pressure versus reciprocal temperature for dihexyl phthalate.

15.1.3.10 Butyl-2-ethylhexyl phthalate (BOP)

Common Name: Butyl-2-ethylhexyl phthalate

Synonym: BEHP, BOP

Chemical Name: Butyl-2-ethylhexyl phthalate

CAS Registry No: 85-69-8

Molecular Formula: $C_{20}H_{30}O_4$, $(C_4H_9OOC)C_6H_4(COOCH_2CH(C_2H_5)(CH_2)_3CH_3)$

Molecular Weight: 333.450

Melting Point ($^{\circ}C$):

-37 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

446.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

< 1.0 (shake flask-HPLC/UV spec., Howard et al. 1985)

0.11; 0.02 (recommended; calculated-QSAR, Staples et al. 1997)

0.075 (calculated-UNIFAC, Thomsen et al. 1999)

0.385 (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

1.47×10^{-5} ; 3.2×10^{-3} , 0.016 (recommended; calculated-QSAR, Staples et al. 1997)

5.37×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0405 (recommended, Staples et al. 1997)

0.466 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.93 (av. from OECD, Howard et al. 1985)

3.70–7.88 (calculated-HPLC-RT, Howard et al. 1985)

6.28; 6.5 (recommended, calculated-QSAR, Staples et al. 1997)

6.20 (calculated-UNIFAC, Thomsen & Carlsen 1998)

5.64 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

9.37 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

6.30 (suspended solids, Staples et al. 1997)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photolysis rate $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a)Oxidation: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0 \text{ d}$ (calculated, Staples et al. 1997).

Hydrolysis:

 $k(\text{second-order alkaline}) = (1.1 \pm 0.1) \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ for pH 10–12 at 30°C, with $t_{1/2}(\text{calc}) = 2000 \text{ yr}$ at pH 7 (calculated as per Radding et al. 1977, Callahan et al. 1979) $k(\text{acid catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{second order alkaline}) = 0.4 \text{ M}^{-1} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a) $k(\text{second-order alkaline}) = (1.1 \pm 0.1) \times 10^{-4} \text{ M}^{-1} \text{ s}^{-1}$ at 30°C in water with $t_{1/2} = 100\text{--}2000 \text{ yr}$ (Wolfe et al. 1980b)Biodegradation: primary biodegradation rate constant $k = 0.153 \text{ d}^{-1}$ and $t_{1/2} = 4.55 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

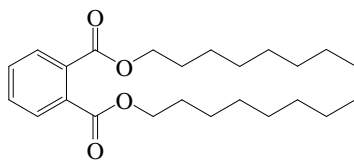
Air: atmospheric photooxidation $t_{1/2} = 0.4\text{--}4.0 \text{ d}$ (calculated, Staples et al. 1997).Surface water: hydrolysis $t_{1/2} = 100\text{--}2000 \text{ yr}$ (Wolfe et al. 1980b; Callahan et al. 1979);primary biodegradation rate constant $k = 0.153 \text{ d}^{-1}$ and $t_{1/2} = 4.55 \text{ d}$ in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.11 Di-*n*-octyl phthalate (DOP)

Common Name: Di-*n*-octyl phthalate

Synonym: di-*n*-octyl phthalate, DOP, *o*-benzenedicarboxylic acid dioctyl ester, *n*-dioctyl phthalate, octyl phthalate, dioctyl-*o*-benzenedicarboxylate

Chemical Name: di-*n*-octyl phthalate

CAS Registry No: 117-84-0

Common Molecular Formula: $C_{24}H_{38}O_4$, $C_6H_4(COOC_8H_{17})_2$

Molecular Weight: 390.557

Melting Point ($^{\circ}C$):

−25.0 (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982; Lide 2003)

Boiling Point ($^{\circ}C$):

220.0 (Patty 1963; Fishbein & Albro 1972; Callahan et al. 1979; Mabey et al. 1982)

Density (g/cm^3 at $20^{\circ}C$):

0.978 (Fishbein & Albro 1972; Ellington 1999)

Molar Volume (cm^3/mol):

399.3 ($20^{\circ}C$, calculated-density)

524.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated):

50.0	($20^{\circ}C$, Fishbein & Albro 1972)
3.0	(shake flask-GC, Wolfe et al. 1979)
3.0	(shake flask-GC, Wolfe et al. 1980a,b)
0.285	($24^{\circ}C$, tech. grade, Verschueren 1983)
0.022	(generator column-HPLC/UV, DeFoe et al. 1990)
0.020, 0.040	(synthesized phthalates by turbidity inflection-HPLC/UV, DeFoe et al. 1990)
1.96	(calculated-molar volume, Wang et al. 1992)
0.0005	(recommended, Staples et al. 1997)
0.00051; 0.00049	(shake flask: slow stirring; no-stirring, GC/FID, Ellington 1999)
0.0092	(calculated-UNIFAC method, Thomsen et al. 1999)
0.0249	(calculated-QSPR, Cousins & Mackay 2000)
0.00040	($20^{\circ}C$, shake flask-GC/MS, Letinski et al. 2002)
0.00040, 0.00042	(QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

4.21×10^{-6}	($20^{\circ}C$, tensimeter, extrapolated, measured range 113 – $162^{\circ}C$, Perry & Weber 1949)
$\log(P/\mu mHg) = 14.68 - 5620/(T/K)$; temp range 113 – $162^{\circ}C$ (tensimeter, Perry & Weber 1949)
0.0187	(estimated by analogy to Henry's law constant, Mabey et al. 1982)
2.92×10^{-5}	(extrapolated-Antoine eq., Stephenson & Malanowski 1987)
$\log(P_L/kPa) = 9.897 - 5197.4/(T/K)$; temp range: 423 – 523 K, (Antoine eq., Stephenson & Malanowski 1987)
1.33×10^{-5}	(recommended, Staples et al. 1997)
2.52×10^{-5}	(calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant (Pa m^3/mol at $25^{\circ}C$):

0.557	(calculated-P/C, Wolfe et al. 1980a)
1.722	(calculated-P/C, Mabey et al. 1982)
0.0297	(quoted from WERL Treatability Data, Ryan et al. 1988)

- 10.435 (selected, Staples et al. 1997)
 0.0249 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 9.2 (calculated as per Leo et al. 1971, Callahan et al. 1979)
 9.2 (calculated, Wolfe et al. 1979)
 8.06 (HPLC-RT correlation; McDuffie 1981)
 8.92 (calculated-CLOGP for synthesized phthalate, DeFoe et al. 1990)
 5.22 (shake flask, $\log P$ database, Hansch & Leo 1987)
 8.06 (recommended, Staples et al. 1997)
 6.99 (calculated-UNIFAC method, Thomsen et al. 1999)
 7.73 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

- 10.53 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

- 2.82, 3.97, 0.064, 3.72, 2.64 (in lab. model ecosystem after 3 d: alga, daphnia, mosquito fish, mosquito larvae, snails, Sanborn et al. 1975)
 4.45, 3.41, 3.97, 3.97, 4.13 (in lab. model ecosystem after 33 d: alga, daphnia, mosquito fish, mosquito larvae, snails, Sanborn et al. 1975)
 3.46 (bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
 8.59 (microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.28 (calculated, Wolfe et al. 1980a)
 9.56 (sediment-water, calculated- K_{OW} , Mabey et al. 1982)
 7.91 (sediment, calculated- K_{OW} , Pavlou & Weston 1983, 1984)
 7.60 (calculated- K_{OW} , Kollig 1993)
 6.30 (suspended solids, calculated- K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)

Environmental Fate Rate Constant, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photolysis rate $k_p = 2 \times 10^{-4} \text{ h}^{-1}$ (EXAMS model, Wolfe et al. 1980a)

Oxidation: $k = 18 \text{ M s}^{-1}$, free radical oxidation rate constant in an aquatic environment (Wolfe et al. 1980a)

$k \ll 360 \text{ M}^{-1} \text{ h}^{-1}$ for singlet oxygen and $k = 1.4 \text{ M}^{-1} \text{ h}^{-1}$ for peroxy radical (Mabey et al. 1982)

photooxidation $t_{1/2} = 4.5\text{--}44.8 \text{ h}$ in air, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Howard et al. 1991)

photooxidation $t_{1/2} = 0.3\text{--}3.0 \text{ d}$ from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997)

$k_{OH} = 20.581 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.40 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

phthalates are susceptible to alkaline hydrolysis, with theoretical $t_{1/2} = 4 \text{ months to } 100 \text{ yr}$ at pH 8 and 30°C (Wolfe et al. 1980a)

$k(\text{acid catalyzed}) = 0.04 \text{ M}^{-1} \text{ h}^{-1}$, $k(\text{second order alkaline}) = 59 \text{ M}^{-1} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a)

$k(\text{base}) = 7.4 \text{ M}^{-1} \text{ h}^{-1}$ at pH 7 and 25°C (Ellington et al. 1987)

$t_{1/2} = 107 \text{ yr}$ at pH 7, $t_{1/2} = 1 \text{ yr}$ at pH 9 and 25°C (Howard et al. 1991; selected, Staples et al. 1997).

Biodegradation: the pseudo first-order degradation rate constant $k = 0.14 \text{ d}^{-1}$ corresponding to $t_{1/2} = 5 \text{ d}$ in a model ecosystem (Sanborn et al. 1975);

degradation $t_{1/2} = 8 \text{ d}$ by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

rate constant $k \sim (1.57 \pm 0.17) \times 10^2 \text{ min}^{-1}$ from retention times of reverse phase chromatography (estimated, Urushigawa & Yonezawa 1979);

microbial degradation rate constant $k = 2 \times 10^{-4} \text{ h}^{-1}$ in an aquatic environment (Wolfe et al. 1980a)

significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate $k < 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);

biodegradation rate constant $k = 7.4 \times 10^{-9} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{d}^{-1}$ at 30°C in water (Scow 1982);

aqueous aerobic $t_{1/2} = 168\text{--}672 \text{ h}$, based on unacclimated and acclimated aqueous screening test data; aqueous anaerobic $t_{1/2} = 4320\text{--}8760 \text{ h}$, based on acclimated anaerobic screening test data (Howard et al. 1991);

rate constant $k = 0.0014 \text{ h}^{-1}$ with $t_{1/2} = 513.4 \text{ h}$ for microbial degradation by anaerobic sludge (Wang et al. 2000)

aerobic biodegradation in aquatic environments, first order $k = 0.7 \text{ d}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ in river water (Peterson & Staples 2003)

anaerobic biodegradation, first order rate $k = 0.006\text{--}0.0336 \text{ d}^{-1}$ with $t_{1/2} = 115\text{--}20.6 \text{ d}$ in undiluted digester sludge of different DOP concn, batch incubation (Peterson & Staples 2003)

Biotransformation: $k = 3.1 \times 10^{-10} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a);

microbial transformation $k = (3.7 \pm 0.6) \times 10^{-13} \text{ L} \cdot \text{organism}^{-1} \cdot \text{h}^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$k_2 = 3.69 \times 10^{-5} \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 3.16 \times 10^{-6} \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} = 4.5\text{--}44.8 \text{ h}$, based on estimated rate constant for the vapor phase reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

photodegradation $t_{1/2} = 0.40 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: degradation $t_{1/2} = 5 \text{ d}$ in an aquatic model ecosystem (Sanborn et al. 1975);

overall degradation $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

biodegradation $t_{1/2} = 1.0 \text{ d}$ in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 336\text{--}8760 \text{ h}$, based on estimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment:

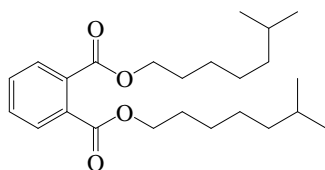
Soil: degradation $t_{1/2} = 8 \text{ d}$ by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

$t_{1/2} = 10\text{--}50 \text{ d}$ via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

degradation $t_{1/2} = 168\text{--}672 \text{ h}$, based on estimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

Biota:

15.1.3.12 Di-isooctyl phthalate (DIOP)



Common Name: Di-isooctyl phthalate

Synonym: DIOP

Chemical Name:

CAS Registry No: 27554-26-3

Molecular Formula: $C_{24}H_{38}O_4$

Molecular Weight: 390.557

Melting Point ($^{\circ}C$):

−4 (Fishbein & Albro 1972)

−46 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

270 (Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

524.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.09 (shake flask-GC, Howard et al. 1985)

0.001; 0.00024, 0.00081 (recommended; calculated-QSAR, Staples et al. 1997)

2.49×10^{-3} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

1.55×10^{-4} (dew-point and tensimeter methods, extrapolated from Clausius-Clapeyron eq., Werner 1952)

$\log(P/\text{micron}) = -4829/(T/K) + 13.262$; temp range 70 – $210^{\circ}C$, (exptl. data fitted to the Clausius-Clapeyron eq., Werner 1952)

7.4×10^{-4} (gas saturation method, Howard et al. 1985)

$\log(P/\text{mmHg}) = 24.8803 - 5.5821 \times 10^3/(T/K) - 1.2116 \cdot \log(T/K) - 1.547 \times 10^{-2} \cdot (T/K) + 6.5101 \times 10^{-6} \cdot (T/K)^2$; temp range 260 – 851 K (vapor pressure eq., Yaw et al. 1994)

1.55×10^{-4} , 7.4×10^{-4} , 4.53×10^{-5} (quoted, Staples et al. 1997)

7.5×10^{-4} ; 1.33×10^{-4} , 2.67×10^{-8} , 1.87×10^{-4} (recommended; calculated-QSAR, Staples 1997)

2.52×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

3.95 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.0; 8.39 (recommended; calculated-QSAR, Staples et al. 1997)

7.73 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.53 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, log BCF:

Sorption Partition Coefficient, log K_{OC} :

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.3\text{--}3.0$ d (Estimated, Staples et al. 1997).

Hydrolysis: aqueous hydrolysis $t_{1/2} \sim 157$ yr (estimated, Staples et al. 1997).

Biodegradation: primary biodegradation rate constant $k = 0.082\text{ d}^{-1}$ and $t_{1/2} = 8.82$ d in an acclimated shake flask
CO₂ evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.3\text{--}3.0$ d (estimated, Staples et al. 1997).

Surface water: primary biodegradation rate constant $k = 0.082\text{ d}^{-1}$ and $t_{1/2} = 8.82$ d in an acclimated shake flask
CO₂ evolution test (Sugatt et al. 1984);

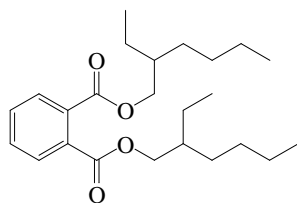
aqueous hydrolysis $t_{1/2} \sim 157$ yr (estimated, Staples et al. 1997).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.13 *bis*-(2-Ethylhexyl) phthalate (DEHP)

Common Name: Di-(2-ethylhexyl) phthalate

Synonym: DEHP, bis(2-ethylhexyl) phthalate, di-(2-ethylhexyl)orthophthalate, bis(2-ethylhexyl) phthalic acid ester, di-*sec*-octyl phthalate, 2-ethylhexyl phthalate, 1,2-benzenedicarboxylic acid bis(2-ethylhexyl) ester

Chemical Name: bis(2-ethylhexyl) phthalate, di-*sec*-octyl phthalate, 2-ethylhexyl phthalate

CAS Registry No: 117-81-7

Molecular Formula: $C_{24}H_{38}O_4$, o - $C_6H_4(COOCH_2CH(C_2H_5)C_4H_9)_2$

Molecular Weight: 390.557

Melting Point ($^{\circ}C$):

-55.0 (Verschuereen 1983; Lide 2003)

Boiling Point ($^{\circ}C$):

384.0 (Dean 1985; Riddick et al. 1986; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

0.9850 (Fishbein & Albro 1972)

0.9843 (Riddick et al. 1986)

Molar Volume (cm^3/mol):

396.1 ($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)

524.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

107.1, 105.9 (Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

100 ($20^{\circ}C$, Fishbein & Albro 1972)

50.0 (from Monsanto Chemical Co. data sheets, Peakall 1975)

0.60 (Branson 1978; Kenaga & Goring 1980)

0.285 (shake flask-nephelometry on technical grade DEHP, Hollifield 1979)

100 (quoted from Metcalf & Lu 1973, Hollifield 1979; Garten & Trabalka 1983)

2.49 (Neely 1979; quoted, Neely & Blau 1985; Lyman 1985; Elzerman & Coates 1987)

0.40 (shake flask-GC, Wolfe et al. 1979, 1980a, b)

1.16 (solubility in 35 L instant ocean solution, Giam et al. 1980)

0.047 (from OECD 1979/80, Klöpffer et al. 1982)

0.041 ($20^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

0.34 ± 0.04 (shake flask-HPLC/UV, Howard et al. 1985)

< 100 (quoted, Riddick et al. 1986)

0.27; 0.36 (centrifugation method, turbidity inflection method, DeFoe et al. 1990)

9.8×10^{-6} to 0.633 (lit. values, Sabljic et al. 1990)

0.003 (recommended, Staples et al. 1997)

0.0249 (calculated-QSPR, Cousins & Mackay 2000)

0.017 ($22^{\circ}C$, shake flask-surface tension measurement, Thomsen et al. 2001)

0.0019 ($20^{\circ}C$, shake flask-GC/MSD, Letinski et al. 2002)

0.00285, 0.00024 (QSAR estimates-SPARC model, WSKOWWIN model, Letinski et al. 2002)

Vapor Pressure (Pa at 25°C or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

- 1.45×10^{-5} (20°C, extrapolated, tensimeter, measured range 95–145°C, Hickman et al. 1937)
- $\log(P/\mu\text{mHg}) = 15.116 - 5590/(T/K)$; temp range 95–145°C (Hickman et al. 1937)
- 1.93×10^{-5} (effusion method, extrapolated-Antoine eq., Small et al. 1948)
- $\log(P/\text{mmHg}) = 12.12 - 5590/(T/K)$ (Antoine eq., quoted from Barclay & Butler 1938; Small et al. 1948)
- $\log(P/\text{mmHg}) = 12.47 - 5757/(T/K)$; pressure range 5×10^{-2} to 10^{-4} mmHg (effusion, data presented in graph and Antoine eq., Small et al. 1948)
- 1.51×10^{-5} (20°C, extrapolated, tensimeter, measured range 99–148°C, Perry & Weber 1949)
- $\log(P/\mu\text{mHg}) = 14.62 - 5440/(T/K)$; temp range 99–148°C (pendulum tensimeter method, Perry & Weber 1949)
- $8.26 \times 10^{-6*}$ (measured by dew-point and tensimeter methods, temp range 120–225°C, extrapolated from Antoine eq., Werner 1952)
- $\log(P/\text{micron}) = 12.639 - 3811/(201.2 + t/^{\circ}\text{C})$; temp range 120–225°C (Antoine eq., Dew-Point and Tensimeter methods, data presented in graph, Werner 1952)
- 2.70×10^{-5} (20°C, calculated-Antoine eq., Weast 1972–73)
- 1.73×10^{-5} (submicron droplet evaporation, Chang & Davis 1976)
- 5.81×10^{-5} (36°C, submicron droplet evaporation, Davis & Ray 1977)
- 5.84×10^{-6} (17°C, submicron droplet evaporation, measured range 17–31°C, Ray et al. 1979)
- $\log(P/\text{mmHg}) = 12.729 - 5822/(T/K)$; temp range 17–31°C (submicron droplet evaporation, Ray et al. 1979)
- $6.0 \times 10^{-6*}$, 1.30×10^{-5} (20°C, effusion-vapor pressure balance, gas saturation method, OECD 1981)
- $\log(P/\text{mmHg}) = 10.086 - 5010.357/(T/K)$; temp range 10–50°C (Antoine eq., gas saturation, OECD 1981)
- $\log(P/\text{mmHg}) = 13.243 - 6035.017/(T/K)$; temp range 80–120°C (Antoine eq., effusion, OECD 1981)
- 5.50×10^{-6} (20°C, estimated-evaporation rate, Dobbs & Cull 1982)
- 7.01×10^{-8} (20°C, gas saturation, measured range 120–140°C, Potin-Gauthier et al. 1982)
- $\log(P/\text{mmHg}) = 18.408 - 8112.265/(T/K)$; temp range 120–140°C (Potin-Gauthier et al. 1982)
- 0.00293, 1.87×10^{-6} , 7.47×10^{-4} (estimation-structure based methods, Tucker et al. 1983)
- $8.6 \pm 6.6 \times 10^{-4}$ (gas saturation-HPLC/UV, Howard et al. 1985)
- 70, 700 (literature values, Riddick et al. 1986)
- 5.08×10^{-5} (extrapolation-Antoine eq., Stephenson & Malanowski 1987)
- $\log(P_L/\text{kPa}) = 11.8564 - 6416.2/(36.74 + T/K)$; temp range 373–660 K (Antoine eq., Stephenson & Malanowski 1987)
- $(1.20\text{--}2.40) \times 10^{-5}$ (quoted from OECD interlaboratory studies, Hinckley et al. 1990)
- 1.90×10^{-5} (GC-RT correlation, Hinckley et al. 1990)
- $1.2 \times 10^{-4*}$ (40°C, OECD Vapour Pressure Curve Guideline 104, temp range 40–80°C, OECD 1993)
- $\log(P/\text{mmHg}) = -0.7422 - 7.2012 \times 10^3/(T/K) + 9.9887 \cdot \log(T/K) - 2.2697 \times 10^{-2} \cdot (T/K) + 8.2181 \times 10^{-6} \cdot (T/K)^2$; temp range 350–886 K (vapor pressure eq., Yaw et al. 1994)
- $1.50 \times 10^{-4*}$ (40°C, Knudsen effusion with different orifice diameters and variable cell height, measured range 40–80°C, Goodman 1997)
- $\log(P/\text{Pa}) = 14.90 - 5911/(T/K)$; temp range 40–80°C (Knudsen effusion, Goodman 1997)

Henry's Law Constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$ at 25°C):

- 0.0446 (calculated-P/C, Wolfe et al. 1980a)
- 1.1140 (calculated, Lyman et al. 1982)
- 0.0304 (20–25°C, calculated-P/C, Mabey et al. 1982)
- 0.0263, 3.14 (calculated-P/C, calculated-group contribution, Tucker et al. 1983)
- 0.0042 (estimated-P/C, Lyman 1985)
- 0.101 (estimated as per Hine & Mookerjee 1975, Lyman 1985)
- 0.0041 (calculated-P/C, Mackay 1985, Neely & Blau 1985)
- 0.0297 (quoted from WERL Treatability Data, Ryan et al. 1988)
- 1.4940 (calculated-P/C, Meylan & Howard 1991)
- 1.1970 (estimated-bond contribution, Meylan & Howard 1991)
- 1.7324 (selected, Staples et al. 1997)
- 3.95 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, log K_{OW} :

3.58	(Lu & Metcalf 1975)
4.20	(Mayer 1976)
5.30	(Hirzy et al. 1978)
8.73	(calculated, Wolfe et al. 1979)
5.11, 4.66–5.45	(shake flask method: mean, range, OECD 1981)
7.86	(HPLC-extrapolated from alkylbenzenes, Harnish et al. 1983)
5.03	(shake flask average, OECD/EEC lab. comparison tests, Harnish et al. 1983)
9.64	(quoted lit. calculated value, Leyder & Boulanger 1983)
7.94	(HPLC-RT correlation, Howard et al. 1985)
7.80, 8.90	(HPLC-RT correlation, TLC-RT, Klein et al. 1988)
7.453 \pm 0.061	(slow-stirring-GC, De Bruijn et al. 1989)
5.22	(shake flask method, Brooke et al. 1990)
7.86, 9.68	(HPLC method, calculated, Brooke et al. 1990)
7.137 \pm 0.153	(stir-flask method by BRE, Brooke et al. 1990)
7.453 \pm 0.061	(stir-flask method by RITOX, Brooke et al. 1990)
7.88	(recommended, Sangster 1993)

Octanol/Air Partition Coefficient, log K_{OA} :

10.53	(calculated-QSPR, Cousins & Mackay 2000)
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Bioconcentration Factor, log BCF:

2.11	(fish, Metcalf et al. 1973)
5.03	(mosquito larvae, Metcalf et al. 1973)
4.13, 3.49, 3.72, 3.36, 2.36	(scud, midge larvae, waterflea, mayfly, sowbug, Sanders et al. 1973)
3.56, 2.54, 2.62, 2.76, 2.66	(scud, midge, waterflea, mayfly, fathead minnow, 14-d exposure, Mayer & Sanders 1973)
3.14	(fathead minnow, 28-d exposure, Mayer & Sanders 1973)
2.76	(fathead minnow, 56-d exposure, Mayer 1976)
2.93	(fathead minnow, Veith et al. 1979)
2.90, 2.15	(fathead minnow, Branson 1978)
2.06	(bluegill sunfish, Barrows et al. 1980)
–1.92	(adipose tissue of female Albino rats, Geyer et al. 1980)
3.95	(bacteria, calculated- K_{OW} , Wolfe et al. 1980a)
0.84–1.05, 1.01–1.22, 1.03–1.13	(oyster, shrimp, fish, Wofford et al. 1981)
1.04	(oyster, Wofford et al. 1981; quoted, Zaroogian et al. 1985)
2.93, 2.88	(fish: quoted, calculated- K_{OW} , Mackay 1982)
2.32	(<i>Daphnia magna</i> , Brown & Thompson 1982a)
3.37, 3.42, 3.40	(mussel <i>Mytilus edulis</i> , Brown & Thompson 1982b)
8.36	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
2.49, 2.11	(fish: flowing water, microcosm conditions, Graten & Trabalka 1983)
3.73, 3.57	(alga <i>Chlorella</i> , calculated- K_{OW} , Geyer et al. 1984)
2.80	(sheephead minnows, predicted-pharmacokinetic model, Karara & Hayton 1984)
2.66, 3.73, 3.48	(golden orfe, algae, activated sludge, Freitag et al. 1982)
1.60, 3.73, 3.48	(golden ide, algae, activated sludge, Freitag et al. 1985)
2.96, 2.87	(oyster, estimated values, Zaroogian et al. 1985)
2.96, 2.87	(sheephead minnows, estimated values, Zaroogian et al. 1985)
2.76	(quoted, Isnard & Lambert 1989)
0.204–1.71	(rainbow trout, BCF to decline as body wt. increased, Tarr et al. 1990)
2.94	(fish, highest fish BCF, Matthiessen et al. 1992)

Sorption Partition Coefficient, log K_{OC} :

4.0–5.0	(soil, calculated values, Kenaga 1980; Wolfe et al. 1980a)
4.756	(sediment-water, calculated- K_{OW} and S, Wolfe et al. 1980a)
9.301	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)

- 4.31, 5.27, 4.90, 4.98 (estimated- K_{OW} , Karickhoff 1985)
 4.24, 5.06 (estimated-S, Karickhoff 1985)
 5.10 (best estimate, expected at low sediment concn. of $< 10^{-4}$ /mL, Karickhoff 1985)
 5.00 (soil/sediment, Neely & Blau 1985)
 4.94 (Broome County soil in New York, shake flask-GC, Russell & McDuffie 1986;)
 5.22 (soil, calculated- MCI χ and fragment contribution, Meylan et al. 1992)
 2.60 (activated carbon, calculated-MCI χ , Blum et al. 1994)
 7.13 (calculated- K_{OW} , Kolliig 1993)
 4.34, 6.00 (suspended solids, calculated- K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

- Volatilization: calculated evaporation rate $k = 0.00052$ cm/h corresponding to $t_{1/2} = 132600$ h for a pond of 1 m deep (Branson 1978).
- Photolysis: rate constant for direct photolysis $k = 2 \times 10^{-4}$ h $^{-1}$ in natural water (Wolfe et al. 1980a);
 $t_{1/2} \sim 143$ d in water is estimated to be 143 d (Wolfe et al. 1980a; quoted, Howard 1989);
 atmospheric $t_{1/2} = 3500$ –4800 h and aqueous $t_{1/2} = 3500$ –4800 h, based on measured rate of aqueous photolysis for DMP (Howard 1991).
 Aqueous photolysis $k = 0.9$ h $^{-1}$ and $t_{1/2} = 0.75$ h (Jin et al. 1999, quoted, Peterson & Staples 2003)
- Oxidation: the free radical oxidation rate constant $k = 18$ M \cdot s $^{-1}$ (Wolfe et al. 1980b);
 photooxidation $t_{1/2} = 44$ –584 d in water, based on estimated rate constant for the reaction with hydroxyl radicals in water (Wolfe et al. 1980; quoted, Howard et al. 1991);
 rate constant $k \ll 360$ M $^{-1}$ ·h $^{-1}$ for singlet oxygen and $k = 7.2$ M $^{-1}$ ·h $^{-1}$ for peroxy radical (Mabey et al. 1982);
 photooxidation $t_{1/2} = 2.9$ –29 h in air, based on estimated rate constant for the reaction with hydroxyl radicals in air (Atkinson 1987; quoted, Howard et al. 1991);
 predicted atmospheric photooxidation $t_{1/2} = 0.2$ –2.0 d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).
 $k_{OH} = 21.955 \times 10^{-12}$ cm 3 molecule $^{-1}$ s $^{-1}$ and $t_{1/2} = 0.38$ d based on a global, seasonal and diurnal average OH radical concn of 1×10^6 molecule cm $^{-3}$ in air (Peterson & Staples 2003)
- Hydrolysis: second order alkaline hydrolysis rate constant $k = 1.1 \times 10^{-4}$ M $^{-1}$ ·s $^{-1}$ for pH 10–12 at 30°C in water (Wolfe et al. 1979, 1980b; quoted, Callahan et al. 1979);
 $t_{1/2} = 100$ to 2000 yr for hydrolytic degradation alone in the eutrophic lake ecosystem at steady-state increase (Wolfe et al. 1980a);
 $t_{1/2}(\text{calc}) = 2000$ yr at pH 7 in water (calculated per Radding et al. 1977; quoted, Callahan et al. 1979; Howard 1989; Howard et al. 1991);
 $k(\text{exptl.}) = 9.5 \times 10^{-7}$ d $^{-1}$ at pH 7 and 25°C while estimated rate constant $k = 1.46 \times 10^{-6}$ d $^{-1}$ at pH 7 and 30°C (Neely 1985);
 first-order hydrolysis $t_{1/2} = 2000$ yr at pH 7, based on measured base catalyzed hydrolysis rate constant (Howard et al. 1991; selected, Staples et al. 1997).
- Biodegradation: approximately calculated rate constant $k = 0.091$ d $^{-1}$ in pond water plus sediment incubated under aerobic conditions based on time for 50% degradation (Johnson & Lulves 1975; quoted, Klečka 1985);
 estimated biodegradation $t_{1/2} \sim 4$ –5 wk by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);
 degradation $t_{1/2} = 1.3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977);
 rate constant $k = 0.023$ d $^{-1}$ in river water incubated under aerobic conditions (Klečka 1985);
 rate constant $k(\text{mineralization rate divided by initial substrate concn.}) = 0.028 \pm 0.013$ d $^{-1}$ in lake water incubated under aerobic conditions (Subba-Rao et al. 1982; quoted, Klečka 1985);
 $t_{1/2} = 2.0$ –3.0 wk, based on river die-away test data (Hattori et al. 1975; Saeger & Tucker 1976; Wolfe et al. 1980; estimated, Howard 1989);
 $t_{1/2} = 0.8$ d in activated sludge (Saeger & Tucker 1976; estimated, Howard 1989);
 microbial degradation rate constant $k = 4.2 \times 10^{-12}$ mL·organism $^{-1}$ ·s $^{-1}$ (Wolfe et al. 1980a);
 significant degradation with gradual adaptation from 7 to 21 d in an aerobic environment with a rate $k < 0.5$ d $^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);
 aqueous aerobic $t_{1/2} = 120$ –550 h, based on grab sample die-away test data (Schouten et al. 1979 and Johnson & Lulves 1975; estimated, Howard et al. 1991); aqueous anaerobic $t_{1/2} = 980$ –9336 h, based on anaerobic

die-away test data (Howard et al. 1991) and anaerobic aqueous screening studies (Horowitz et al. 1982 and Shelton et al. 1984; estimated, Howard et al. 1991);
mean rate constant $k = 0.136 \text{ d}^{-1}$ corresponding to $t_{1/2} = 5.25 \text{ d}$ in shake flask biodegradation experiment (Sugatt et al. 1984);

more than 90% of initial 3.3 mg/L will be degraded in activated sludge systems in 2–5 d (O'Grady et al. 1985);

greater than 50% loss in microbial degradation in less than 20 d under aerobic conditions, very low under anaerobic conditions in garden soil (Shanker et al. 1985);

readily metabolized in uninoculated Erie slit loam with the absence of nonaqueous-phase liquids (NAPLs) for about 20 d (Efroymson & Alexander 1994)

biphasic microbial mineralization kinetics: $k = 0.0044 \text{ d}^{-1}$ with $t_{1/2} = 158 \text{ d}$ at 5°C , $k = 0.0081 \text{ d}^{-1}$ with $t_{1/2} = 86 \text{ d}$ at 10°C , and $k = 0.0134 \text{ d}^{-1}$ with $t_{1/2} = 52 \text{ d}$ at 20°C in agriculture soil for phase I; and $t_{1/2} = 224 \text{ d}$ at 5°C , $t_{1/2} = 187 \text{ d}$ at 10°C and $t_{1/2} = 73 \text{ d}$ at 20°C in agriculture soil for phase II. Rate $k = 0.0023 \text{ d}^{-1}$ with $t_{1/2} = 301 \text{ d}$ at 5°C , $k = 0.0055 \text{ d}^{-1}$ with $t_{1/2} = 125 \text{ d}$ at 10°C , and $k = 0.0127 \text{ d}^{-1}$ with $t_{1/2} = 55 \text{ d}$ at 20°C in sludge-amended soil for phase I and $t_{1/2} \geq 365 \text{ d}$ at 5°C , $t_{1/2} = 337 \text{ d}$ at 10°C and $t_{1/2} = 150 \text{ d}$ at 20°C in sludge-amended soil for phase II kinetics in laboratory microcosms. At 20°C , aerobic mineralization rate $k = 0.0182 \text{ d}^{-1}$ with $t_{1/2} = 37 \text{ d}$ for phase I, $t_{1/2} = 51 \text{ d}$ for phase II in well-mixed sludge, $k = 0.0058 \text{ d}^{-1}$ with $t_{1/2} = 120 \text{ d}$ for phase I, $t_{1/2} \geq 365 \text{ d}$ for phase II in aggregate sludge, aerobic $k = 0.0127 \text{ d}^{-1}$ with $t_{1/2} = 55 \text{ d}$ for phase I, $t_{1/2} = 150 \text{ d}$ for phase II and anaerobic $k = 0.0023 \text{ d}^{-1}$ with $t_{1/2} = 301 \text{ d}$ for phase I, $t_{1/2} \geq 365 \text{ d}$ for phase II in sludge-amended soil (Madsen et al. 1999).

aerobic biodegradation in aquatic environments, first order $k = 0.023 \text{ d}^{-1}$ with $t_{1/2} = 30 \text{ d}$ in unstirred river water, $k = 0.2 \text{ d}^{-1}$ with $t_{1/2} = 3.5 \text{ d}$ in shaken river water, $k = 1.73 \text{ d}^{-1}$ with $t_{1/2} = 0.4 \text{ d}$ field data, estuarine sediment (Peterson & Staples 2003)

aerobic soil degradation, pseudo-first-order $k = 0.035 \text{ d}^{-1}$ with $t_{1/2} = 2.0 \text{ d}$ in loam; $k = 0.010 \text{ d}^{-1}$ with $t_{1/2} = 69.3 \text{ d}$ in sand; $k = 0.033 \text{ d}^{-1}$ with $t_{1/2} = 21 \text{ d}$ in outdoor lysimeter, loam; $k = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53.3 \text{ d}$ in outdoor lysimeter, sand; $k = 0.12 \text{ d}^{-1}$ with $t_{1/2} = 5.6 \text{ d}$ in garden soil; $k = 0.040 \text{ d}^{-1}$ with $t_{1/2} = 17.3 \text{ d}$ in soil with 2% OC-organic carbon; $k = 0.019 \text{ d}^{-1}$ with $t_{1/2} = 36.5 \text{ d}$ in soil with 3.3% OC; $k = 0.015 \text{ d}^{-1}$ with $t_{1/2} = 46.2 \text{ d}$ in soil with 1.6% OC and $k = 0.012 \text{ d}^{-1}$ with $t_{1/2} = 58 \text{ d}$ in sludge amended loam. For anaerobic degradation, first order rate $k > 0.3 \text{ d}^{-1}$ with $t_{1/2} < 2.3 \text{ d}$ in undiluted digester sludge, batch incubation; $k = 0.013 \text{ d}^{-1}$ with $t_{1/2} = 53.3 \text{ d}$ in flood soil; $k = 0.69 \text{ d}^{-1}$ with $t_{1/2} = 1.0 \text{ d}$ field data, sediment (Peterson & Staples 2003)

Biotransformation: $k = 4.2 \times 10^{-12} \text{ mL} \cdot \text{cell}^{-1} \cdot \text{h}^{-1}$ for bacterial transformation in water (Wolfe et al. 1980a; quoted, Mabey et al. 1982);

microbial transformation $k = (4.2 \pm 0.7) \times 10^{-15} \text{ L} \cdot \text{organism}^{-1} \cdot \text{h}^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

$t_{1/2} = 7 \text{ d}$ for elimination of DEHP from fathead minnows (Mayer & Sanders 1973);

fish elimination $t_{1/2} = 6.2$ to 18.3 d with a mean value of 12.2 d after 56 d exposure period (fathead minnows, Mayer 1976);

$k_1 = 76 \text{ mL g}^{-1} \cdot \text{h}^{-1}$ (fish, Branson 1978);

depuration $t_{1/2} = 72 \text{ h}$ (tissues of bluegill sunfish, Barrows et al. 1980).

$k_2 = 3.69 \times 10^{-5} \text{ d}^{-1}$ (10°C , 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 3.16 \times 10^{-6} \text{ d}^{-1}$ (10°C , 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} =$ half-life of 2.9–29 h, based on estimated rate constant for the reaction with hydroxyl radicals in air (Howard et al. 1991);

atmospheric transformation lifetime was estimated to be $< 1 \text{ d}$ (Kelly et al. 1994).

Photodegradation $t_{1/2} = 0.38 \text{ d}$ based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} \sim 4$ to 5 wk in river water by naturally occurring, mixed microbial populations (Saeger & Tucker 1976);

$t_{1/2} = 5 \text{ d}$ in a model ecosystem (Verschuere 1983);

$t_{1/2} = 5.25 \text{ d}$ in an acclimated shake flask CO_2 evolution biodegradation experiment (Sugatt et al. 1984)

$t_{1/2} = 120$ – 550 h , based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991)

Biodegradation $t_{1/2} = 0.3\text{--}30$ d in estuarine river water with sediment and river water (Peterson & Staples 2003)

Ground water: $t_{1/2} = 240\text{--}9336$ h, based on unacclimated aqueous aerobic and anaerobic biodegradation half-life (Howard et al. 1991).

Sediment:

Soil: degradation $t_{1/2} = 1.3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977) biodegradation $t_{1/2} < 20$ d under anaerobic conditions in a garden soil (Shanker et al. 1985);

$t_{1/2} = 10\text{--}50$ d via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

degradation $t_{1/2} = 39$ d for initial phase, $t_{1/2} = 51$ d for the late phase in sludge-amended quartz; $t_{1/2} = 58$ d for initial phase and $t_{1/2} = 147$ d for sludge-amended soil, $t_{1/2} = 58$ d for initial phases and $t_{1/2} = 84$ d in sludge slurry; $t_{1/2} = 9$ d for initial phases, $t_{1/2} = 35$ d for late phase in sludge-amended soil + strain SDE-2 (Roslev et al. 1998)

overall $t_{1/2} = 120\text{--}550$ h, based on unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

degradation by microorganism in biometer systems, $t_{1/2} = 66$ d in silty sand standard metabolism experiments, $t_{1/2} = 102$ d corrected standard conditions, $t_{1/2} = 170$ d in simulated outdoor conditions; $t_{1/2} = 20$ d in silty loam standard conditions, $t_{1/2} = 30$ d corrected standard conditions, $t_{1/2} = 31$ d in simulated outdoor conditions at constant soil moisture and 20°C ; degradation by microorganism in outdoor experiments in small lysimeter systems: $t_{1/2} = 54$ d outdoor fallow and $t_{1/2} = 200$ d outdoor barley in silty sand, and $t_{1/2} = 21$ d outdoor fallow, $t_{1/2} = 14$ d outdoor barley in silty loam (Rüdel et al. 1993)

microbial mineralization $t_{1/2} = 158, 86$ and 52 d at $5, 10$, and 20°C , respectively, in soil; $t_{1/2} = 301, 125$ and 55 d at $5, 10$ and 20°C in sludge-amended soil in phase I degradation kinetics; $t_{1/2} = 224, 187$ and 73 d at $5, 10$, and 20°C , respectively, in soil; $t_{1/2} = 365, 337$ and 150 d at $5, 10$ and 20°C in sludge-amended soil in phase II degradation kinetics. At 20°C , $t_{1/2}$ varies between $77\text{--}89$ d and $100\text{--}127$ d for phase I and II, respectively, in sludge-amended soil with different initial DEHP concns. Aerobic $t_{1/2} = 37$ d and 51 d for phase I and II in well mixed sludge, $t_{1/2} = 120$ d and > 365 d for phase I and II in aggregate sludge, $t_{1/2} = 55$ d and 150 d for phase I and II in sludge-amended soil; anaerobic $t_{1/2} = 301$ d and > 365 d for phase I and II in sludge-amended soil (laboratory microcosms, Madsen et al. 1999)

biodegradation in aerobic soil: $t_{1/2} = 2.0\text{--}69.3$ d in various sand, loam, soils with different organic carbon content and sludge amended loam in laboratory and outdoor experiments (Peterson & Staples 2003)

Biota: elimination and degradation $t_{1/2} < 4$ d after 7 d for water fleas *Daphnia magna* and $t_{1/2} = 7$ d for fathead minnows (Mayer & Sanders 1973);

fish elimination $t_{1/2} = 12.2$ d (fathead minnows *Pimephales promelas*, Mayer 1976);

depuration $t_{1/2} = 3$ d (in tissues of bluegill sunfish continuously for 42-d exposure, Barrows et al. 1980)

depuration $t_{1/2} = 38$ d from sheephead minnow (Karara & Hayton 1984).

TABLE 15.1.3.13.1

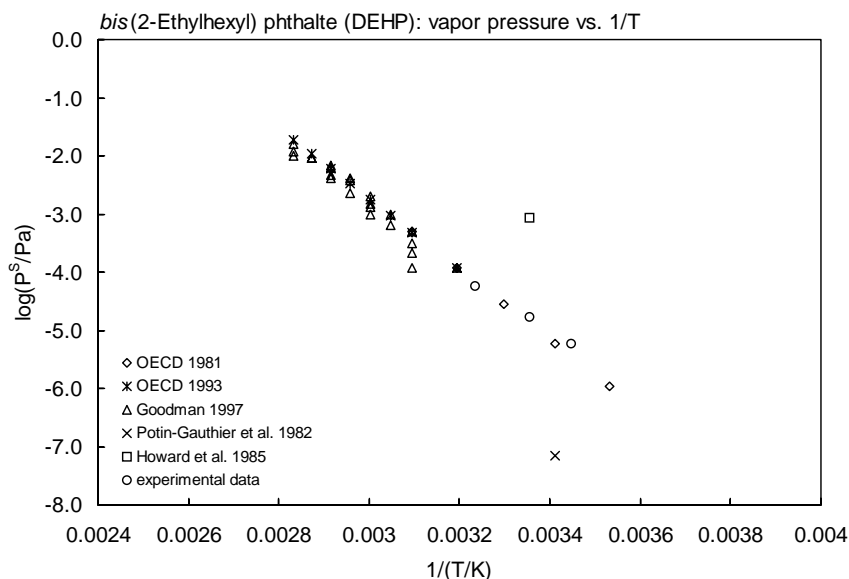
Reported vapor pressures of *bis*(2-ethylhexyl) phthalate (DEHP) at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^\circ\text{C})$		(2)	$\ln P = A - B/(C + t/^\circ\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
OECD 1981		OECD 1993		Goodman 1997	
effusion/gas saturation		v.p. curve guideline 104		Knudsen effusion	
$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa	$t/^\circ\text{C}$	P/Pa
effusion-vapor pres. balance				orifice diameter 0.381 mm	
10	1.1×10^{-6}	40	1.2×10^{-4}	50	1.2×10^{-4}
20	6.0×10^{-6}	50	4.8×10^{-4}	50	3.1×10^{-4}
30	2.8×10^{-5}	55	9.3×10^{-4}	55	9.8×10^{-4}
40	1.2×10^{-4}	60	1.8×10^{-3}	55	6.5×10^{-4}
				using variable cell height	
				50	2.1×10^{-4}
				60	9.7×10^{-4}
				65	4.1×10^{-3}

(Continued)

TABLE 15.1.3.13.1 (Continued)

OECD 1981		OECD 1993		Goodman 1997			
effusion/gas saturation		v.p. curve guideline 104		Knudsen effusion		Knudsen effusion	
t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
50	4.9×10^{-4}	65	3.3×10^{-3}	60	2.0×10^{-3}	70	6.8×10^{-3}
		70	5.9×10^{-3}	60	1.3×10^{-3}	75	9.2×10^{-3}
eq. 1	P/Pa	75	0.011	65	3.8×10^{-3}	80	1.0×10^{-2}
A	13.243	80	0.019	65	2.3×10^{-3}	40	1.2×10^{-4}
B	6035.017			70	6.3×10^{-3}	50	4.9×10^{-4}
				70	4.2×10^{-3}	60	1.5×10^{-3}
				75	9.2×10^{-3}	70	4.6×10^{-3}
gas saturation				80	0.012	80	1.6×10^{-2}
10	1.1×10^{-6}	Small et al. 1948					
20	6.0×10^{-6}	effusion method					
30	2.8×10^{-5}	t/°C	P/Pa			eq. 1	P/Pa
40	1.2×10^{-4}					A	14.90
50	4.9×10^{-4}	data presented in graph and				B	5911
		eq. 1	P/mmHg				
eq. 1	P/Pa	A	12.47				
A	10.086	B	5757				
B	5010.357	for pressure range: 0.05 to					
		10^{-4} mmHg					

FIGURE 15.1.3.13.1 Logarithm of vapor pressure versus reciprocal temperature for *bis*(2-ethylhexyl) phthalate.

15.1.3.14 Di(hexyl,octyl,decyl) phthalate

Common Name: Di(hexyl,octyl,decyl) phthalate

Synonym: 610P

Chemical Name:

CAS Registry No: 25724-58-7, 68515-51-5

Molecular Formula: $C_{25}H_{40}O_4$

Molecular Weight: 404.583

Melting Point ($^{\circ}C$):

−4 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

547.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.9 ± 0.5 (shake flask, Howard et al. 1985)

0.05; 0.0004 (recommended; calculated-QSAR, Staples et al. 1997)

8.76×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

6.5×10^{-4} (gas saturation, Howard et al. 1985)

6.5×10^{-4} ; 4.53×10^{-5} , 6.5×10^{-2} (recommended; calculated-QSAR, Staples et al. 1997)

1.31×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

6.05 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.9–8.61 (HPLC-RT correlation, Howard et al. 1985; quoted, Staples et al. 1997)

7.25; 8.54 (recommended; calculated-QSAR, Staples et al. 1997)

8.17 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

10.78 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2$ – 4.0 d (estimated, Staples et al. 1997).

Hydrolysis:

Biodegradation: primary biodegradation with a rate constant $k = 0.131$ d^{-1} and $t_{1/2} = 5.30$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}4.0$ d (estimated, Staples et al. 1997).

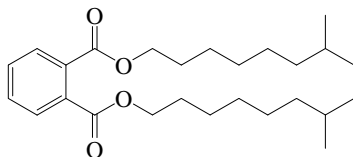
Surface water: primary biodegradation with a rate constant $k = 0.131\text{ d}^{-1}$ and $t_{1/2} = 5.30$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil:

Biota:

15.1.3.15 Diisononyl phthalate (DINP)

Common Name: Diisononyl phthalate

Synonym: DINP

Chemical Name:

CAS Registry No: 28553-12-0, 68515-48-0

Molecular Formula: $C_{26}H_{42}O_4$

Molecular Weight: 418.609

Melting Point ($^{\circ}C$):

-48 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

413 (Fishbein & Albro 1972)

Density (g/cm^3 at $20^{\circ}C$):

0.995 (Fishbein & Albro 1972)

Molar Volume (cm^3/mol):

569.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.20 ± 0.1 (shake flask-GC, Howard et al. 1985)

0.20, 0.0006 (quoted, Staples et al. 1997)

< 0.001 ; 7.8×10^{-5} , 2.3×10^{-5} (recommended; calculated-QSAR, Staples et al. 1997)

3.08×10^{-4} (calculated-QSPR, Cousins & Mackay 2000)

6.1×10^{-4} ($20^{\circ}C$, shake flask/slow stirring-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$):

7.2×10^{-5} (gas saturation method, Howard et al. 1985)

6.67×10^{-5} ; 1.33×10^{-8} , 3.07×10^{-5} (recommended; calculated-QSAR, Staples et al. 1997)

6.81×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

9.26 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

> 8.0 ; 9.0, 9.4 (recommended; calculated-QSAR, Staples et al. 1997)

8.60 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.03 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

3.27 (*Arca zebra*, Solbakken et al. 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

$k_{OH} = 23.408 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.35$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation with a rate constant $k = 0.131 \text{ d}^{-1}$ and $t_{1/2} = 5.31$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 848 \text{ mL} \cdot \text{g} \cdot \text{d}^{-1}$ (*Arca zebra*, 26.5°C , Solbakken et al. 1985; quoted, Staples et al. 1997)

$k_2 = 0.46 \text{ d}^{-1}$ (*Arca zebra*, 26.5°C , Solbakken et al. 1985; quoted, Staples et al. 1997)

$k_2 = 0.02 \text{ d}^{-1}$ (*Diplora strigosa*, 26.5°C , Solbakken et al. 1985; quoted, Staples et al. 1997)

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

Photodegradation $t_{1/2} = 0.35$ h based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: primary biodegradation with a rate constant $k = 0.131 \text{ d}^{-1}$ and $t_{1/2} = 5.31$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

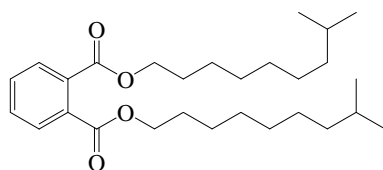
Groundwater:

Sediment:

Soil:

Biota:

15.1.3.16 Di-isodecyl phthalate (DIDP)



Common Name: Di-isodecyl phthalate

Synonym: DIDP

Chemical Name: di-diisodecyl phthalate

CAS Registry No: 26761-40-0, 68515-49-1

Molecular Formula: $C_{28}H_{46}O_4$

Molecular Weight: 446.663

Melting Point ($^{\circ}C$):

- 48 (Stephenson & Malanowski 1987)
- 46 (Staples et al. 1997)
- 50 (Lide 2003)

Boiling Point ($^{\circ}C$):

- 450 (Stephenson & Malanowski 1987)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

- 464.8 (Stephenson & Malanowski 1987)
- 613.6 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

- < 50 (quoted from Monsanto Chemical Co. data sheets, Peakall 1975)
- 1.19 ± 0.19 (shake flask-GC, Howard et al. 1985)
- 0.28 (shake flask-nephelometry, Hollifield 1979)
- 0.19, 0.28, < 0.00013 (quoted, Staples et al. 1997)
- < 0.001; 2.2×10^{-6} , 7.4×10^{-6} (recommended, calculated-QSAR, Staples et al. 1997)
- 3.81×10^{-5} (calculated-QSPR, Cousins & Mackay 2000)
- 1.7×10^{-4} ($20^{\circ}C$, shake flask/slow stirring-GC/MS, Letinski et al. 2002)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

- $\log(P_L/kPa) = 14.0158 - 10984/(242.24 + T/K)$, temp range: 371–496 K, (Antoine eq., Stephenson & Malanowski 1987)
- $\log(P/mmHg) = 81.7895 - 7.4225 \times 10^3/(T/K) - 26.916 \cdot \log(T/K) + 1.1502 \times 10^{-2} \cdot (T/K) - 4.353 \times 10^{-14} \cdot (T/K)^2$; temp range 233–723 K (vapor pressure eq., Yaw et al. 1994)
- 6.67×10^{-5} , 7.47×10^{-5} (quoted, Staples et al. 1997)
- 6.67×10^{-5} ; 6.67×10^{-6} , 4.93×10^{-6} , 1.33×10^{-8} (recommended, calculated-QSAR, Staples et al. 1997)
- 1.84×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

- 21.6 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 7.70 (estimated, Williams et al. 1995)
- > 8.0; 10.0, 1.0.3 (recommended; calculated-QSAR, Staples et al. 1997)
- 9.46 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

11.52 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

1.95–2.1, 2.06 (*Daphnia magna*, 20°C, range, mean, Brown & Thompson 1982a)

3.48, 3.60; 3.54 (*Mytilus edulis*, 15°C, exposure concn: 4.4, 4.17 µg/L; mean value, Brown & Thompson 1982b)

Sorption Partition Coefficient, $\log K_{OC}$:

5.04, 5.78, 5.16 (soil/sediment, exptl. data, Williams et al. 1995)

5.46, 7.60 (soil/sediment: mean value, calculated- K_{OW} , Williams et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2$ – 2.0 d (estimated, Staples et al. 1997).

$k_{OH} = 26.217 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.32$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 4.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);

primary biodegradation with a rate constant $k = 0.088 \text{ d}^{-1}$ and $t_{1/2} = 9.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 795, 539 \text{ mL} \cdot \text{g} \cdot \text{d}^{-1}$ (*Mytilus edulis*, for exposure concn: 4.4, 4.17 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).

$k_2 = 0.20, 0.18 \text{ d}^{-1}$ (*Mytilus edulis*, for exposure concn: 4.4, 4.17 µg/L, 15°C, Brown & Thompson 1982b; quoted, Staples et al. 1997).

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2$ – 2.0 d (estimated, Staples et al. 1997).

photodegradation $t_{1/2} = 0.32$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

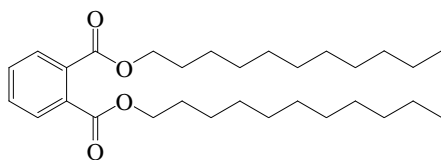
Surface water: primary biodegradation with a rate constant $k = 0.088 \text{ d}^{-1}$ and $t_{1/2} = 9.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 4.0$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota: depuration $t_{1/2} = 3.5$ and 3.8 d DIDP concn at 5 and 50 µg/L for *Mytilus edulis* at 15°C (Brown & Thompson 1982b).

15.1.3.17 Diundecyl phthalate (DUP)

Common Name Diundecyl phthalate

Synonym: DUP

Chemical Name: diundecyl phthalate

CAS Registry No: 3648-20-2

Molecular Formula: $C_{30}H_{50}O_4$

Molecular Weight: 474.716

Melting Point ($^{\circ}C$):

-9 (Staples et al. 1997)

35.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.96 (Staples et al. 1997)

Molar Volume (cm^3/mol):

658.0 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.789 (mp at $35.5^{\circ}C$)

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.11 ± 0.28 (shake flask, Howard et al. 1985)

< 0.001 ; 1.6×10^{-7} , 4.2×10^{-7} (recommended; calculated-QSAR, Staples et al. 1997)

2.14×10^{-8} (calculated-UNIFAC, Thomsen et al. 1999)

4.41×10^{-6} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

6.67×10^{-5} , 7.07×10^{-5} (quoted, Staples et al. 1997)

6.67×10^{-5} ; 1.33×10^{-8} , 1.6×10^{-7} (recommended; calculated-QSAR, Staples et al. 1997)

4.97×10^{-7} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

50.5 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

> 8.0 ; 11.2, 11.5 (recommended; calculated-QSAR, Staples et al. 1997)

10.54 (calculated-UNIFAC, Thomsen et al. 1999)

10.33 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

12.02 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{oc}$:

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

$k_{\text{OH}} = 31.847 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.26$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis:

Biodegradation: primary biodegradation rate constant $k = 0.115 \text{ d}^{-1}$ and $t_{1/2} = 6.17$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

aerobic biodegradation in aquatic environments, first order $k = 0.03 \text{ d}^{-1}$ with $t_{1/2} = 23$ d in unstirred river water (Peterson & Staples 2003)

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997)

Photodegradation $t_{1/2} = 0.26$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: primary biodegradation rate constant $k = 0.115 \text{ d}^{-1}$ and $t_{1/2} = 6.17$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

biodegradation $t_{1/2} = 23$ d in aerobic aquatic environments (Peterson & Staples 2003)

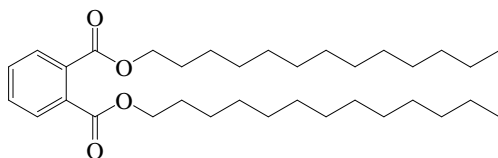
Groundwater:

Sediment:

Soil:

Biota:

15.1.3.18 Ditridecyl phthalate (DTDP)



Common Name: Ditridecyl phthalate

Synonym: DTDP

Chemical Name:

CAS Registry No: 119-06-2. 68515-47-9

Molecular Formula: $C_{34}H_{58}O_4$

Molecular Weight: 530.823

Melting Point ($^{\circ}C$):

-37 (Staples et al. 1997)

Boiling Point ($^{\circ}C$):

Density (g/cm^3 at $20^{\circ}C$):

0.953 (Staples et al. 1997)

Molar Volume (cm^3/mol):

746.8 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.34 (shake flask-nephelometry, Hollifield 1979)

< 0.30 (shake flask, Howard et al. 1985; quoted, Adams et al. 1995)

0.34, < 0.30 (quoted, Staples et al. 1997)

< 0.001; 1.5×10^{-9} , 4.2×10^{-9} (recommended, calculated-QSAR, Staples et al. 1997)

4.07×10^{-10} (calculated-UNIFAC, Thomsen et al. 1999)

7.0×10^{-8} (calculated-QSPR, Cousins & Mackay 2000)

Vapor Pressure (Pa at $25^{\circ}C$):

< 6.67×10^{-5} (quoted, Staples et al. 1997)

< 6.67×10^{-5} ; 1.33×10^{-9} , 3.33×10^{-9} (recommended; calculated-QSAR, Staples et al. 1997)

3.63×10^{-8} (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

275 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

8.40 (estimated, Williams et al. 1995)

> 8.0; 13.1, 13.4 (recommended; calculated-QSAR, Staples et al. 1997)

12.28 (calculated-UNIFAC, Thomsen et al. 1999)

12.06 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

13.01 (calculated-QSPR, Cousins & Mackay 2000)

Bioconcentration Factor, $\log BCF$:

Sorption Partition Coefficient, $\log K_{OC}$:

6.08 (soil/sediment, Williams et al. 1995; quoted, Staples et al. 1997)

5.87, 6.45, 6.28; 6.08 (soil/sediment: exptl. data; mean value, Williams et al. 1995)

6.26, 8.30 (soil/sediment: exptl. mean, calculated- K_{OW} , Williams et al. 1995)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

Hydrolysis:

Biodegradation: degradation $t_{1/2} = 10.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977);

primary biodegradation rate constant $k = 0.029\text{ d}^{-1}$ and $t_{1/2} = 27.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air: atmospheric photooxidation $t_{1/2} \sim 0.2\text{--}2.0$ d (estimated, Staples et al. 1997).

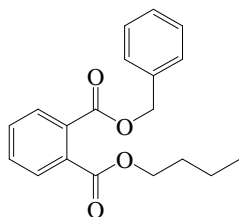
Surface water: primary biodegradation rate constant $k = 0.029\text{ d}^{-1}$ and $t_{1/2} = 27.6$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984).

Groundwater:

Sediment:

Soil: degradation $t_{1/2} = 10.5$ d by microorganisms (*Pseudomonas acidovorans* 256–1) from soil or waste water at 30°C (Kurane et al. 1977).

Biota:

15.1.3.19 Butyl benzyl phthalate (BBP)

Common Name: Butyl benzyl phthalate

Synonym: BBP, benzyl butyl phthalate

Chemical Name: butyl benzyl phthalate, benzyl butyl phthalate

CAS Registry No: 85-68-7

Molecular Formula: $C_{19}H_{20}O_4$, $C_6H_5COOCH_2C_6H_4COOC_4H_9$

Molecular Weight: 312.360

Melting Point ($^{\circ}C$):

–35.0 (Callahan et al. 1979; Mabey et al. 1982; Howard 1989)

Boiling Point ($^{\circ}C$):

370.0 (Verschuereen 1983; Howard 1989; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.111 (Staples et al. 1997)

Molar Volume (cm^3/mol):

369.2 (calculated-Le Bas method at normal boiling point)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.90 (Hirzy et al. 1978)

0.71 (shake flask-nephelometry, practical grade, Hollifield 1979)

2.9 ± 1.2 (shake flask-GC, Gledhill et al. 1980)

40.2 (shake flask-LSC, Veith et al. 1980)

2.82 ($20^{\circ}C$, shake flask-UV, Leyder & Boulanger 1983)

2.90 ± 1.2 (Verschuereen 1983)

2.69 ± 0.15 (shake flask-HPLC/UV, Howard et al. 1985)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

0.00115 ($20^{\circ}C$, Gledhill et al. 1980)

0.00799 (calculated using Trouton's rule, Mabey et al. 1982)

0.00115 (Petrasek et al. 1983)

0.00115 ($20^{\circ}C$, Verschuereen 1983)

$\log(P_L/kPa) = 9.1472 - 4647.5/(T/K)$, temp range: 416–516 K, (Antoine eq., Stephenson & Malanowski 1987)

0.0011, 0.00133 (quoted, calculated-solvatochromic parameters and UNIFAC, Banerjee et al. 1990)

0.00067 (recommended, Staples et al. 1997)

0.0249 (calculated-QSPR, Cousins & Mackay 2000)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.132 (calculated-P/C, Wolfe et al. 1980a)

0.132 (calculated, Lyman et al. 1982)

0.841 (calculated-P/C, Mabey et al. 1982)

0.104 (quoted from WERL Treatability Data, Ryan et al. 1988)

0.077 (selected, Staples et al. 1997)

0.205 (calculated-QSPR, Cousins & Mackay 2000)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.80	(Hirzy et al. 1978)
5.80	(calculated as per Leo et al. 1971)
4.77	(shake flask-GC analysis of both phases, Gledhill et al. 1980)
4.05	(shake flask-LSC, Veith et al. 1980; Veith & Kosian 1982)
4.75	(RPHPLC-RT correlation, Veith et al. 1980)
3.97	(HPLC- k' correlation, McDuffie 1981)
4.11, 3.23–4.45	(shake flask method: mean, range, OECD 1981)
4.91	(20°C, shake flask-UV, Leyder & Boulanger 1983)
4.78	(Verschuereen 1983)
3.57	(HPLC-RT correlation, Howard et al. 1985)
4.91	(calculated, Hansch & Leo 1985)
4.87	(calculated-CLOGP, Müller & Klein 1992)
4.59	(recommended, Staples et al. 1997)
4.70	(calculated-QSPR, Cousins & Mackay 2000)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

8.78	(calculated-QSPR, Cousins & Mackay 2000)
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Bioconcentration Factor, $\log BCF$:

2.74–3.34	(calculated- K_{OW} , Veith et al. 1979, 1980)
2.82	(bluegill sunfish, Barrows et al. 1980;)
2.71	(calculated- K_{OW} , Gledhill et al. 1980)
2.82	(bluegill sunfish, quoted, Gledhill et al. 1980)
2.19–2.95	(fathead minnows, quoted, Gledhill et al. 1980)
2.89	(bluegill sunfish, Veith et al. 1980; Veith & Kosian 1982)
3.90	(calculated- K_{OW} , Wolfe et al. 1980a)
4.67	(microorganisms-water, calculated- K_{OW} , Mabey et al. 1982)
3.57	(sediment, calculated- K_{OW} , Pavlou & Weston 1983, 1984)
2.89	(quoted, Isnard & Lambert 1988; quoted, Banerjee & Baughman 1991)
2.72	(calculated- K_{OW} and $S_{octanol}$, Banerjee & Baughman 1991)

Sorption Partition Coefficient, $\log K_{OC}$:

1.83–2.54	(soil, batch equilibration-GC, Gledhill et al. 1980;)
3.95	(soil/sediment, Gledhill et al. 1980)
3.81	(calculated- K_{OW} , Wolfe et al. 1980a)
5.23	(sediment-water, calculated- K_{OW} , Mabey et al. 1982)
4.23	(Broome County soil in New York, Russell & McDuffie)
4.23, 3.97	(soil, quoted, calculated-MCI and fragment contribution, Meylan et al. 1992)
2.60	(activated carbon, calculated-MCI, Blum et al. 1994)
3.21	(quoted or calculated-QSAR MCI $^1\chi$, Sabljic et al. 1995)
5.00	(suspended solids, calculated- K_d assuming a 0.1 org. carbon fraction, Staples et al. 1997)
3.21, 3.88; 3.11, 3.07, 3.21, 3.32, 3.15	(soil: quoted lit., calculated- K_{OW} ; HPLC-screening method using LC-columns of different stationary phases, Szabo et al. 1999)

Environmental Fate Rate Constants, k , and Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis: direct photolysis (near surface) rate constant $k = 2 \times 10^{-4} \text{ h}^{-1}$ in natural water (Wolfe et al 1980a); photodegradation $t_{1/2} > 100 \text{ d}$ (Gledhill et al. 1980; quoted, Verschuereen 1983; Howard 1989).

Oxidation: the free radical oxidation rate constant $k = 18 \text{ M}^{-1}\text{s}^{-1}$ for reaction with peroxy radical (Wolfe et al. 1980a);

rate constant $k \ll 360 \text{ M}^{-1}\text{h}^{-1}$ for singlet oxygen and $k = 280 \text{ M}^{-1}\text{h}^{-1}$ for peroxy radical (Mabey et al. 1982); photooxidation $t_{1/2} = 6\text{--}60 \text{ h}$, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991);

predicted atmospheric photooxidation $t_{1/2} = 0.5\text{--}5.0$ d from Atkinson 1988 atmospheric-oxidation program (Staples et al. 1997).

$k_{\text{OH}} = 11.049 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $t_{1/2} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Hydrolysis: the alkaline hydrolysis rate constant $k \sim 38 \text{ M}^{-1}\cdot\text{h}^{-1}$; hydrolytic $t_{1/2} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

chemical degradation (hydrolysis) $t_{1/2} > 100$ d (Gledhill et al. 1980; quoted, Verschuere 1983; Howard 1989; selected, Staples et al. 1997).

Biodegradation: degradation $t_{1/2} \sim 2$ d in river water and $t_{1/2} = 2$ h in activated sludge (Saeger & Tucker 1976)

degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

microbial degradation rate constant $k = 2.9 \times 10^{-8} \text{ mL}\cdot\text{organism}^{-1}\cdot\text{s}^{-1}$ (Wolfe et al. 1981a);

0–24% mineralization in > 8 wk in municipal digested sludge (Horowitz et al. 1982);

primary degradation accounted for > 95% loss in 7 d with an initial concentration of 1.0 mg/L in a lake water microcosm with $t_{1/2} < 4$ d and 100% primary degradation was observed after 9 d while $t_{1/2} = 2.0$ d (Gledhill et al. 1980; quoted, Verschuere 1983; Howard 1989);

significant degradation with rapid adaptation within 7 d in an aerobic environment with $k > 0.5 \text{ d}^{-1}$ (Tabak et al. 1981; quoted, Mills et al. 1982);

degradation rate constant $k = 0.043 \text{ d}^{-1}$ corresponding to $t_{1/2} = 19.4$ d in a shake flask biodegradation experiment (Sugatt et al. 1984);

greater than 90% degraded within 40 d in digested sludge (Shelton et al. 1984);

99% degraded in activated sludge systems in 48 h (O'Grady et al. 1985);

anaerobic digestion of sludge with first-order rate constant $k = 6.5 \times 10^{-3} \text{ h}^{-1}$ and $t_{1/2} = 107$ h (Ziougou et al. 1989);

aqueous aerobic $t_{1/2} = 24\text{--}168$ h, based on unacclimated river die-away test and aqueous anaerobic $t_{1/2} = 672\text{--}4320$ h, based on unacclimated anaerobic screening test data (Howard et al. 1991)

Aerobic biodegradation in aquatic environments, first order $k = 0.46 \text{ d}^{-1}$ with $t_{1/2} = 1.5$ d in unstirred river water, $k = 0.50 \text{ d}^{-1}$ with $t_{1/2} = 1.4$ d in microcosm, lake, $k = 0.35 \text{ d}^{-1}$ with $t_{1/2} = 2.0$ d in river water, $k = 0.14 \text{ d}^{-1}$ with $t_{1/2} = 5.0$ d in microcosm, un-impacted, $k > 0.023 \text{ d}^{-1}$ with $t_{1/2} < 3.0$ d in microcosm, Illinois river, and $k = 2.2 \text{ d}^{-1}$ with $t_{1/2} = 0.32$ d in shake river water (Peterson & Staples 2003)

Anaerobic biodegradation $k = 0.056 \text{ d}^{-1}$ with $t_{1/2} = 12.4$ d in undiluted sludge, batch incubation, $k = 0.19 \text{ d}^{-1}$ with $t_{1/2} = 3.7$ d in undiluted sludge, $k = 0.096 \text{ d}^{-1}$ with $t_{1/2} = 7.2$ d in 10% dilute sludge; $k = 0.076 \text{ d}^{-1}$ with $t_{1/2} = 9.1$ d in 10% freshwater sediment and $k = 0.051 \text{ d}^{-1}$ with $t_{1/2} = 13.6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Biotransformation: estimated rate constant $k = 3 \times 10^{-9} \text{ mL}\cdot\text{cell}^{-1}\cdot\text{h}^{-1}$ for bacterial transformation in water (Mabey et al. 1982);

microbial transformation $k = (3.1 \pm 0.8) \times 10^{-11} \text{ L}\cdot\text{organism}^{-1}\cdot\text{h}^{-1}$ in natural aquatic systems (Steen et al. 1979; quoted, Steen 1991).

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants or Half-Lives:

depuration $t_{1/2} < 24$ and > 48 h from tissues of bluegill sunfish (Barrows et al. 1980).

$k_2 = 0.0464 \text{ d}^{-1}$ (10°C, 0.1 kg staghorn sculpin, lipid content 5%, Gobas et al. 2003)

$k_2 = 0.00397 \text{ d}^{-1}$ (10°C, 3 kg dogfish, lipid content 15%, Gobas et al. 2003)

Half-Lives in the Environment:

Air: $t_{1/2} = 1.5$ d in the atmosphere (GEMS 1984; quoted, Howard 1989);

$t_{1/2} = 6\text{--}60$ h, based on estimated rate data for the reaction with hydroxyl radical in air (Atkinson 1987; quoted, Howard et al. 1991).

photodegradation $t_{1/2} = 0.75$ d based on a global, seasonal and diurnal average OH radical concn of $1 \times 10^6 \text{ molecule cm}^{-3}$ in air (Peterson & Staples 2003)

Surface water: biodegradation $t_{1/2} \sim 2$ h by naturally occurring, mixed microbial populations in river water (Saeger & Tucker 1976);

hydrolytic $t_{1/2} = 80$ to 4000 d at pH 8 and 30°C (Wolfe et al. 1980a; quoted, Gledhill et al. 1980);

$t_{1/2} = 2$ d for river water, $t_{1/2} < 4$ d for lake water-sediment microcosm, and $t_{1/2} < 100$ d for chemical degradation (hydrolysis) (Gledhill et al. 1980);

biodegradation $t_{1/2} = 19.4$ d in an acclimated shake flask CO_2 evolution test (Sugatt et al. 1984);

overall $t_{1/2} = 24\text{--}168$ h, based on unacclimated river die-away test (Howard et al. 1991)

biodegradation $t_{1/2} = 0.32\text{--}3$ d in aerobic aquatic environments (Peterson & Staples 2003)

Ground water: $t_{1/2} = 48\text{--}4320$ h, based on estimated unacclimated aqueous aerobic and anaerobic biodegradation half-lives (Howard et al. 1991).

Sediment: anaerobic biodegradation $t_{1/2} = 9.1$ h in 10% freshwater sediment, and $t_{1/2} = 13.6$ d in 10% salt marsh sediment (Peterson & Staples 2003)

Soil: degradation $t_{1/2} = 3$ d by microorganisms isolated from soil or waste water at 30°C (Kurane et al. 1977)

$t_{1/2} = 10\text{--}50$ d via volatilization subject to plant uptake from the soil (Ryan et al. 1988);

$t_{1/2} = 24\text{--}168$ h, based on estimated unacclimated aqueous aerobic biodegradation half-life (Howard et al. 1991).

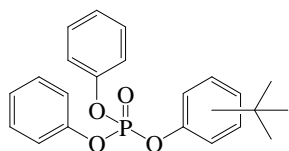
Biota: depuration $t_{1/2} < 24$ and > 48 h (tissues of bluegill sunfish in 21-d exposure, Barrows et al. 1980)

$t_{1/2} < 2$ d from bluegill sunfish (Gledhill et al. 1980; quoted, Verschueren 1983).

15.1.4 PHOSPHATE ESTERS

15.1.4.1 Triaryl phosphates

15.1.4.1.1 *t*-Butylphenyl diphenyl phosphate (tBPDP, BPDP)



Common Name: *t*-Butylphenyl diphenyl phosphate

Synonym: TBPDP, BPDP

Chemical Name:

CAS Registry No: 56803-37-3

o-*tert*-butylphenyl diphenyl phosphate (*o*-TBPDP) 83242-23-2

m-*tert*-butylphenyl diphenyl phosphate (*m*-TBPDP) 83242-22-2

p-*tert*-butylphenyl diphenyl phosphate (*p*-TBPDP) 981-40-8

Molecular Formula: C₂₂H₂₃O₄P, (CH₃)C₆H₄(C₆H₅)₂O₄P

Molecular Weight: 382.389

Melting Point (°C):

−21 (Muir 1984)

Boiling Point (°C):

195/0.20 mmHg, 200/0.2 mmHg, 200/0.20 mmHg (*o*-, *m*-, *p*-TBPDP, Wightman & Malaiyanki 1983)

261/6 mmHg (Muir 1984)

420 (Boethling & Cooper 1985)

Density (g/cm³):

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F: 1.0

Water Solubility (g/m³ or mg/L at 25°C):

3.2 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):

180 (200°C, Muir 1984)

1.87 × 10^{−4} (quoted measured value, Boethling & Cooper 1985)

6.13 × 10^{−5} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.086 (estimated-P/C, Muir 1984, Muir et al. 1985)

0.0223, 0.0073 (calculated-P/C, Boethling & Cooper 1985)

2.18 (gas stripping, Muir et al. 1985)

Octanol/Water Partition Coefficient, log K_{OW}:

5.12 (shake flask-concn ratio, Saeger et al. 1979;)

3.23, 4.76, 6.44; 5.97 (RP-HPLC-*k'* correlation; mean value, Renberg et al. 1980)

Bioconcentration Factor, log BCF:

2.89 (calculated, Saeger et al. 1979)

3.36, 3.04, 3.13 (rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)

2.89 (rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)

3.52, 2.89, 2.70 (fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)

2.76 (fathead minnow, calculated with hexane extract, Muir et al. 1983b)

- 3.94, 2.89 (rainbow trout, fathead minnow, static expt., quoted, Boethling & Cooper 1985)
 3.64 (calculated- K_{OW} , Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

- 4.16 (calculated- K_{OW} , Muir 1984)
 3.36 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 128$ d from 1 m deep water system was estimated to be 128 d (calculated, Muir 1984)
 moderate rate of volatilization from water, $t_{1/2} = 152$ d at 0.5-m depth (Muir et al. 1985).

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 1.92$ h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b).

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 22.8 \text{ h}^{-1}$, 29.3 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_1 = 17.7 \text{ h}^{-1}$, 18.0 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_2 = 0.0137 \text{ h}^{-1}$, 0.0113 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0106 \text{ h}^{-1}$, 0.0111 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

$k_2 = 0.0088 \text{ h}^{-1}$, 0.0074 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0078 \text{ h}^{-1}$, 0.0070 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

hydrolysis $t_{1/2} = 1.92$ h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b);

$t_{1/2} = 128$ d, volatilization from 1 m deep water system (Muir 1984);

pseudo-first-order $t_{1/2} = 0.44$ d in pond water; moderate rate of volatilization from water column with $t_{1/2} = 152$ d at 0.5-m depth (Muir et al. 1985).

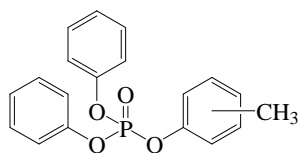
Groundwater:

Sediment: pseudo-first-order $t_{1/2} = 39$ d in pond bottom sediment during a 49-d period (Muir et al. 1985).

Soil:

Biota: depuration $t_{1/2} = 42$ h in chironomid larvae (Muir et al. 1985).

15.1.4.1.2 Cresyl diphenyl phosphate (CDP)



Common Name: Cresyl diphenyl phosphate

Synonym: CDP

Chemical Name:

CAS Registry No: 78-31-9

o-CDP 5254-12-6

m-CDP 69500-28-3

p-CDP 78-31-9

Molecular Formula: C₁₉H₁₇O₄P

Molecular Weight: 340.309

Melting Point (°C):

−40 (*p*-CDP, Lide 2003)

Boiling Point (°C):

180/0.60 mmHg, 190/0.60 mmHg, 200/0.70 mmHg (*o*-, *m*-, *p*-CDP, Wightman & Malaiyandi 1983)

368, 390 (at 1 atm, Boethling & Cooper 1985)

235–255/4 mmHg, 255/5 mmHg (Boethling & Cooper 1985)

Density (g/cm³ at 20°C):

Molar Volume (cm³/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25°C (assuming ΔS_{fus} = 56 J/mol K), F:

Water Solubility (g/m³ or mg/L at 25°C):

2.60 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at 25°C):

5.47×10^{-3} , 1.21×10^{-3} , 3.87×10^{-4} , 2.80×10^{-4} (estimated from reported boiling points, Boethling & Cooper 1985)

6.27×10^{-4} (quoted measured value, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at 25°C):

0.470 (calculated-P/C, Muir 1984)

0.798, 0.162, 0.0820, 0.0507, 0.0355 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW}:

4.505 (shake flask-concn ratio, Saeger et al. 1979)

3.23, 3.63, 4.06; 3.77 (RP-HPLC-*k'* correlation; mean value, Renberg 1980)

4.40 (Bengtsson et al. 1986)

Octanol/Air Partition Coefficient, log K_{OA}:

Bioconcentration Factor, log BCF:

2.56 (calculated, Saeger et al. 1979)

2.99 (calculated-K_{OW}, Boethling & Cooper 1985)

2.002.34 (bleak, 280-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

3.83 (calculated- K_{OW} , Muir 1984)

3.41 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 22$ d for 1 m deep water system (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

volatilization $t_{1/2} = 22$ d for 1 m deep water system (estimated, Muir 1984).

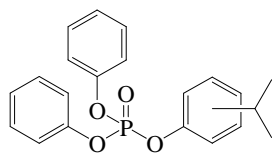
Groundwater:

Sediment:

Soil:

Biota: elimination $t_{1/2} = 4$ d or less (beak, 28-d exposure, Bengtsson 1986).

15.1.4.1.3 Isopropylphenyl diphenyl phosphate (IPDP)



Common Name: Isopropylphenyl diphenyl phosphate

Synonym: IPPDP, IPDP

Chemical Name:

CAS Registry No: 28108-99-8

o-IPPDP 64532-94-1

m-IPPDP 69515-46-4

p-IPPDP 55864-04-5

Molecular Formula: $C_{21}H_{21}O_4P$, $(CH_3)_2CHC_6H_4O_4P$

Molecular Weight: 368.362

Melting Point ($^{\circ}C$):

-26 (Muir 1984)

Boiling Point ($^{\circ}C$):

175/0.05 mmHg, 180/0.02 mmHg, 185/0.05 mmHg (Wightman & Malaiyandi 1983)

220–230/1 mmHg (Muir 1984, Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

2.20 (room temp, shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$):

1.47×10^{-4} (estimated from boiling point, Boethling & Cooper 1985)

3.73×10^{-5} (quoted measured value, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.243, 0.0628 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.305 (shake flask-concn ratio, Saeger et al. 1979; quoted, Muir 1984)

3.23, 4.30, 5.40, 6.57; 5.99 (RP-HPLC- k' correlation; mean, Renberg et al. 1980)

5.70 (quoted measured value, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.99 (calculated, Saeger et al. 1979)

3.88 (estimated from solubility, Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

4.26 (calculated- K_{OW} , Muir 1984)

3.45 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

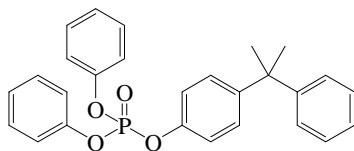
Groundwater:

Sediment:

Soil:

Biota:

15.1.4.1.4 4-Cumylphenyl diphenyl phosphate (CPDPP)



Common Name: 4-Cumylphenyl diphenyl phosphate

Synonym: CPDPP

Chemical Name:

CAS Registry No: 84602-56-2

Molecular Formula: $C_{27}H_{25}O_4P$, $C_6H_5C(CH_3)_2(C_6H_5)_2O_4P$

Molecular Weight: 444.458

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

230–235/0.15 mmHg (Wightman & Malaiyandi 1983)

494 (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.063 ± 0.025 (Mayer et al. 1981)

0.060 (Boethling & Cooper 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

1.726×10^{-9} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

8.62×10^{-4} (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

6.08 (Mayer et al. 1981)

6.10 (quoted, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.40 (calculated- K_{OW} , Mayer et al. 1981)

3.45, 3.10–3.66 (mean value, range, rainbow trout 90-d exposure, Mayer et al. 1981)

4.40 (calculated- K_{OW} , Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

4.53 (soil, calculated-S and K_{OW} , Mayer et al. 1981)

4.30 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: hydrolyzed in alkaline solutions, $t_{1/2} = 5$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

Biodegradation: $t_{1/2} > 21$ d in river die-away procedure; the half-lives of the disappearance by sediment adsorption and degradation of CPDFF for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d, sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in alkaline solutions, $t_{1/2} = 5$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7; biodegradation $t_{1/2} > 21$ d in river die-away procedure (Mayer et al. 1981).

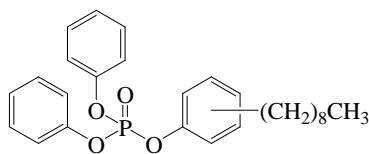
Groundwater:

Sediment: rapidly disappeared from the active core-water columns, 90% in < 3 d in the microcosm-lake simulation study, the half-lives of the disappearance of CPDFF by sediment adsorption and degradation are, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d; sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Soil:

Biota:

15.1.4.1.5 Nonylphenyl diphenyl phosphate (NPDPP)



Common Name: Nonylphenyl diphenyl phosphate

Synonym: NPDPP, Pydral 50E

Chemical Name:

CAS Registry No: 38638-05-0

m-NPDPP 84602-55-1

p-NPDPP 64532-97-4

Molecular Formula: $C_{27}H_{33}O_4P$, $C_9H_{19}(C_6H_5)_3O_4P$

Molecular Weight: 452.522

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

220–225/0.07 mmHg (*m*-NPDPP, Wightman & Malaiyandi 1983)

215–220/0.07 mmHg (*p*-NPDPP, Wightman & Malaiyandi 1983)

471 (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.77 ± 0.25 (Mayer et al. 1981)

0.80 (Boethling & Cooper 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

6.13×10^{-5} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.00142 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.93 (Mayer et al. 1981; quoted, Muir 1984)

5.90 (quoted, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.32 (estimated, Mayer et al. 1981)

2.84, 2.49–2.96 (mean value and range, rainbow trout 90-d exposure, Mayer et al. 1981)

4.26 (calculated- K_{ow} , Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

4.36 (soil, calculated-solubility and K_{ow} , Mayer et al. 1981)

4.61 (calculated- K_{ow} , Muir 1984)

3.69 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, Half-Lives, $t_{1/2}$

Volatilization:

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 6$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

Biodegradation: primary biodegradation $t_{1/2} > 21$ d in river die-away procedure; half-life for disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for core conditions: active, aerated or nitrogen-purge, light or dark $t_{1/2} < 3$ d; sterile, aerated, light $t_{1/2} = 7$ d and sterile, nitrogen-purge, light $t_{1/2} > 28$ d (Mayer et al. 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: hydrolyzed in alkaline solutions, $t_{1/2} = 6$ d at pH 9 and 25°C, but $t_{1/2} > 28$ d at pH 5 and 7 (Mayer et al. 1981).

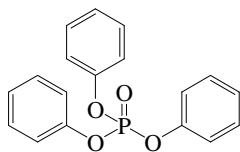
Groundwater:

Sediment: rapidly disappeared from the active core-water column, 90% in < 3 d. Time to 50% disappearance by sediment adsorption and degradation in microcosms-lake simulation study, for microcosm core conditions: active, aerated or nitrogen-purge, light or dark – $t_{1/2} < 3$ d; sterile, aerated, light – $t_{1/2} = 7$ d and sterile, nitrogen-purge, light – $t_{1/2} > 28$ d (Mayer et al. 1981).

Soil:

Biota:

15.1.4.1.6 Triphenyl phosphate (TPP)



Common Name: Triphenyl phosphate

Synonym: TPP

Chemical Name: triphenyl phosphate

CAS Registry No: 115-86-6

Molecular Formula: $C_{18}H_{15}O_4P$

Molecular Weight: 326.283

Melting Point ($^{\circ}C$):

50.5 (Lide 2003)

Boiling Point ($^{\circ}C$):

245/11 mmHg (Verschuereen 1983; Budavari 1989; Lide 2003)

377 (Stephenson & Malanowski 1987)

Density (g/cm^3):

Molar Volume (cm^3/mol):

270.7 ($50^{\circ}C$, Stephenson & Malanowski 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.27, 0.292

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.90 (shake flask-GC, Saeger et al. 1979)

1.9 ± 0.2 (Mayer et al. 1981)

0.73 (shake flask-nephelometry, Hollifield 1979)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

< 13.3 ($30^{\circ}C$, Verschueren 1983)

2.0×10^{-4} , 1.6×10^{-4} , 1.07×10^{-4} (estimated from reported boiling points, Boethling & Cooper 1985)

$\log(P/kPa) = 8.195 - 4253/(T/K)$; temp range 275 – $410^{\circ}C$ (Antoine eq., Stephenson & Malanowski 1987)

$\log(P/mmHg) = 28.0972 - 5.6684 \times 10^3/(T/K) - 5.9768 \cdot \log(T/K) - 3.1567 \times 10^{-9} \cdot (T/K) + 1.0751 \times 10^{-12} \cdot (T/K)^2$;
temp range 323 – 687 K (vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.168 (calculated-P/C, Muir 1984)

0.0265, 0.0284, 0.018 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.63 (shake flask-concn ratio, Saeger et al. 1979)

4.62 (Mayer et al. 1981)

4.78 (shake flask-concn ratio, Sasaki et al. 1981)

3.15 (RP-HPTLC- k' correlation, Renberg et al. 1980)

3.63–3.61 (literature average, Muir 1984)

4.60, 4.70 (Boethling & Cooper 1985)

3.90 (Bengtsson et al. 1986)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$ or $\log K_B$:

2.45, 2.62 (quoted-rainbow trout data, calculated- K_{ow} , Saeger et al. 1979)

2.22 (fathead minnow, mixed isomers, Veith et al. 1979)

3.41	(rainbow trout, rate constant ratio k_1/k_2 , Muir et al. 1980)
3.29, 2.63, 2.58	(rainbow trout, calculated- K_{OW} , Muir et al. 1980)
3.02, 2.92, 2.00	(rainbow trout, calculated-S, Muir et al. 1980)
2.62	(rainbow trout, estimated from K_{OW} , Mayer et al. 1981)
2.43, 2.12–2.56	(mean value, range, rainbow trout in 90-d exposure, Mayer et al. 1981)
2.40–2.79	(killifish, whole fish basis, 72-h exposure, static system, Sasaki et al. 1981)
2.04–2.18	(goldfish, static system, Sasaki et al. 1981; quoted, Boethling & Cooper 1985)
2.20–2.79	(killifish, flow through system, Sasaki et al. 1982; quoted, Boethling & Cooper 1985)
2.28–2.29	(killifish, 32–35 d exposure, flow through system, Sasaki et al. 1983)
3.14, 2.76, 2.96	(rainbow trout: “initial rate” method, static test, Biofac, Muir et al. 1983b)
2.51	(rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
3.24, 2.75, 2.34	(fathead minnow: “initial rate” method, static test, Biofac, Muir et al. 1983b)
2.62	(fathead minnow, calculated with hexane extract, Muir et al. 1983b)
2.76, 2.51	(rainbow trout in static test expt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
2.75, 2.62 1985)	(fathead minnow in static test expt., quoted from Muir et al. 1983b, Boethling & Cooper 1985)
3.26	(estimated- K_{OW} , Boethling & Cooper 1985)
2.60	(bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC} :

3.74	(soil, calculated-S, K_{OW} , Mayer et al. 1981)
3.89	(calculated- K_{OW} , Muir 1984)
3.49	(calculated-solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constant, k, and Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 60$ d (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

$k = 0.0253$ and $0.0227 \text{ L mol}^{-1} \text{ s}^{-1}$ for the colorimetric and acid-base method, respectively, in dioxan-water (3:1 v/v) at 35°C ; the mean second order rate constants: $10^3 k_2$ at 0°C , 10.1°C , 24.7°C , and 35°C were 0.235, 0.477, 1.06, and $2.32 \text{ L mol}^{-1} \text{ s}^{-1}$, respectively, in 60% dioxan-water (Barnard et al. 1961);

$t_{1/2} = 1.3$ yr under neutral conditions from kinetic data in the environment (estimated, Saeger et al. 1979)

$k = 6.0 \times 10^{-8} \text{ s}^{-1}$, with $t_{1/2} = 130$ d, the pseudo-first-order rate constant in dioxan-water (3:1 v/v) at 100°C ; while the second-order rate constant $k = 0.0106 \text{ L mol}^{-1} \text{ s}^{-1}$ with $t_{1/2} = 23$ d at pH 9.5 and $t_{1/2} = 474$ d at pH 8.2 under alkaline conditions at 24.7°C (quoted, Howard & Deo 1979);

$k(\text{second order alkaline}) = 0.027 \text{ M}^{-1} \text{ s}^{-1}$, with an estimated $t_{1/2} \sim 1000$ yr (Wolfe 1980)

$t_{1/2} = 19$ d at pH 7 but $t_{1/2} = 3$ d at pH 9 at 25°C , the most important process for abiotic transformation of aryl phosphates in the environment, much more rapid at alkaline than at neutral pH (Mayer et al. 1981, quoted, Boethling & Cooper 1985)

$t_{1/2} = 7.5$ d at pH 8.2, $t_{1/2} = 1.3$ d at pH 9.5, $t_{1/2} = 20$ –25 d at pH 7 and 21°C (Howard & Deo 1979; quoted, Boethling & Cooper 1985)

$t_{1/2} = 0.49$ h at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b)

Biodegradation: complete primary degradation in less than 7 d in the river die-away studies exposed to the natural microbial population of the river water; $t_{1/2} < 7$ d for primary biodegradation rate for from semicontinuous activated sludge studies (Saeger et al. 1979);

readily biodegraded, in the semicontinuous activated sludge test, degradation of TPP exceeding 95% was observed over a 24-h cycle, and river die-away tests showed $t_{1/2} = 2$ –4 d; time to 50% from the active core water-column disappearance for TPP in microcosms simulating lake conditions was 3–10 d (Mayer et al. 1981).

Biotransformation:

Bioconcentration and Uptake and Elimination Rate Constants (k_1 and k_2):

$k_1 = 46.36 \text{ h}^{-1}$ (rainbow trout, Muir et al. 1980).

$k_2 = 0.0197 \text{ h}^{-1}$ (rainbow trout, 0–9 d, fast clearance, Muir et al. 1980).

$k_2 = 0.00245 \text{ h}^{-1}$ (rainbow trout, 9–31 d, slow clearance, Muir et al. 1980)

- $k_1 = 0.4\text{--}0.6\text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
- $k_1 = 2.1\text{--}4.2\text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
- $k_1 = 3.3\text{--}10.4\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using first-order kinetic and concn factors, Muir et al. 1983)
- $k_1 = 3.3\text{--}16.9\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, 96-h exposure, calculated by using initial uptake data of 0–12 h, Muir et al. 1983)
- $k_2 = 0.023\text{ h}^{-1}$ (*Chironomus tentans* larvae in pond sediment-water system, calculated by concn decay curve, Muir et al. 1983)
- $k_2 = 0.039\text{ h}^{-1}$ (*Chironomus tentans* larvae in river water system, calculated by concentration decay curve, Muir et al. 1983)
- $k_2 = 0.011\text{ h}^{-1}$ (*Chironomus tentans* larvae in river sediment-water system, calculated by concentration decay curve, Muir et al. 1983)
- $k_2 = 0.016\text{ h}^{-1}$ (*Chironomus tentans* larvae in sediment (sand)-water system, calculated by concentration decay curve, Muir et al. 1983).
- $k_1 = 22.7\text{ h}^{-1}$, 20.7 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).
- $k_1 = 16.5\text{ h}^{-1}$, 14.5 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).
- $k_2 = 0.0116\text{ h}^{-1}$, 0.0144 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b)
- $k_2 = 0.0121\text{ h}^{-1}$, 0.0140 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).
- $k_2 = 0.0076\text{ h}^{-1}$, 0.0107 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

$t_{1/2} = 5$ h in the water containing killifish and over 100 h for goldfish (Sasaki et al. 1981);

hydrolysis $t_{1/2} = 19$ d at pH 7 but $t_{1/2} = 3$ d at pH 9; $t_{1/2} = 2\text{--}4$ d in river die-away test at 25°C, (Mayer et al. 1981, quoted, Boethling & Cooper 1985);

$t_{1/2} = 7.5$ d at pH 8.2 and $t_{1/2} = 1.3$ d at pH 9.5, $t_{1/2} = 20\text{--}25$ d at pH 7 at 21°C (Howard & Deo 1979; quoted, Boethling & Cooper 1985);

estimated hydrolysis $t_{1/2} \sim 10^3$ yr (Wolfe 1980);

volatilization $t_{1/2}(\text{calc}) = 60$ d for 1 m deep water (Muir 1984).

Ground water:

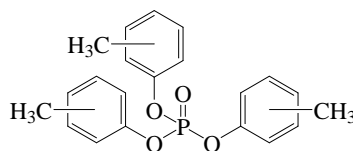
Sediment: water-column disappearance $t_{1/2} \sim 3$ d of TPP by both adsorption and degradation from microcosms-lake simulation study, for the microcosm core conditions: active, aerated, light or dark – $t_{1/2} = 3$ d; active, nitrogen-purge, light – $t_{1/2} = 3$ d; sterile, aerated, light – $t_{1/2} = 7$ d and sterile, nitrogen-purge, light – $t_{1/2} = 10$ d (Mayer et al. 1981).

Soil:

Biota: elimination $t_{1/2} = 30.4$ h in pond sediment-water, $t_{1/2} = 17.6$ h in river water, $t_{1/2} = 62.7$ h in river sediment-water, $t_{1/2} = 44.4$ in sand-water systems (*Chironomus tentans* larvae, Muir et al. 1983a);

elimination $t_{1/2} = 4$ d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

15.1.4.1.7 Tricresyl phosphate (TCP)



Common Name: Tricresyl phosphate

Synonym: TCP, tritolyl phosphate, tris(methylphenyl) phosphate

Chemical Name: phosphoric acid tris(methylphenyl) ester

o-TCP:- tris(2-methylphenyl) phosphate; phosphoric acid tri(2-tolyl) ester

m-TCP:- tris(3-methylphenyl) phosphate; phosphoric acid tri(3-tolyl) ester

p-TCP:- tris(4-methylphenyl) phosphate; phosphoric acid tri(4-tolyl) ester

CAS Registry No:

o-TCP [78-30-8]; *m*-TCP[563-04-2]; *p*-TCP [78-32-0]

mixed isomers - tris(methylphenyl) phosphate [1330-78-5]

Molecular Formula: $C_{21}H_{21}O_4P$, $(CH_3C_6H_4)_3O_4P$

Molecular Weight: 368.362

Melting Point ($^{\circ}C$):

-25/-30	(<i>o</i> -TCP, Verschueren 1983)
-33	(mixed isomers, Riddick et al. 1986)
11, 25-26, 77-8	(<i>o</i> -TCP, <i>m</i> -TCP, <i>p</i> -TCP, Muir 1984)
11, 25, 77.5	(<i>o</i> -TCP, <i>m</i> -TCP, <i>p</i> -TCP, Stephenson & Malanowski 1987)
11, 25.5, 77.5	(<i>o</i> -TCP, <i>m</i> -TCP, <i>p</i> -TCP, Lide 2003)

Boiling Point ($^{\circ}C$):

201/1 mmHg (commercial quality, Burrow 1946)	
420	(<i>o</i> -TCP, Verschueren 1983)
410	(<i>o</i> -TCP, Muir 1984; Lide 2003)
313, 206, 216/0.5 mmHg (mixed isomers, <i>o</i> -, <i>m</i> -TCP, Riddick et al. 1986)	
241-255/4 mmHg, 265/5 mmHg (Boethling & Cooper 1985)	

Density (g/cm^3 at $20^{\circ}C$):

1.159, 1.1718	($25^{\circ}C$, mixture of isomers, <i>o</i> -TCP, Riddick et al. 1986)
1.16	(<i>o</i> -TCP, Verschueren 1983; Riddick et al. 1987; Budavari 1989)

Molar Volume (cm^3/mol):

308.1	($20^{\circ}C$, calculated-density, Stephenson & Malanowski 1987)
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Enthalpy of Vaporization, ΔH_v (kJ/mol):

116.3, 102.9, 113	(<i>m</i> -TCP, Small et al. 1948)
113.4	(<i>p</i> -TCP, Small et al. 1948)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.40	(shake flask-GC, Saeger et al. 1979)
0.074	(<i>p</i> -TCP practical grade, shake flask-nephelometry; Hollifield 1979)
0.36	(mixed isomers, Muir 1984)
< 0.10	(Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.00516-0.00612* (*m*-TCP, Celluloid Corporation samples at $80^{\circ}C$, static and dynamic methods, measured range $80-136^{\circ}C$, Verhoek & Marshall 1939)

$\log(P/\mu mHg) = 15.886 - 6088/(T/K)$; temp range $80-136^{\circ}C$ (*m*-TCP, Celluloid Corporation samples, static and dynamic methods, Verhoek & Marshall 1939)

- 0.0132* (*m*-TCP, Eastman Kodak Co. samples at 85.2°C, static and dynamic methods, measured range 85.2–126°C, Verhoek & Marshall 1939)
 $\log(P/\mu\text{mHg}) = 13.982 - 5373/(T/K)$; temp range 85.2–126°C (*m*-TCP, Eastman Kodak Co. samples, static and dynamic methods, Verhoek & Marshall 1939)
 0.0113* (*p*-TCP, 92°C, static and dynamic methods, measured range 92–145°C, Verhoek & Marshall 1939)
 $\log(P/\mu\text{mHg}) = 15.223 - 5926/(T/K)$; temp range 92–145°C (*p*-TCP, static and dynamic methods, Verhoek & Marshall 1939)
 4.13×10^{-4} (extrapolated from exptl. data, measured range 140–156°C, commercial quality, ebulliometry, Burrows 1946)
 $\log(P/\text{mmHg}) = 12.69 - 5925/(T/K)$; temp range: ~100–150°C (Antoine eq. from exptl., effusion, technical grade, Small et al. 1948)
 $\log(P/\text{mmHg}) = 12.89 - 6088/(T/K)$ (*m*-TCP, Antoine eq. from literature, Small et al. 1948)
 $\log(P/\text{mmHg}) = 10.98 - 5373/(T/K)$ (*m*-TCP, Antoine eq. from literature, Small et al. 1948)
 $\log(P/\text{mmHg}) = 12.22 - 5895/(T/K)$; temp range: 100–150°C (*m*-TCP, Antoine eq., effusion method, data presented in graph and Antoine eq., Small et al. 1948)
 $\log(P/\text{mmHg}) = 12.22 - 5926/(T/K)$ (*p*-TCP, effusion, Antoine eq., Small et al. 1948)
 $\log(P/\mu\text{mHg}) = 14.12 - 5480/(T/K)$; temp range 115–168°C (*p*-TCP, pendulum-tensimeter method, Perry & Weber 1949)
 $\log(P/\text{mmHg}) = [-0.2185 \times 20835.9/(T/K)] + 10.654252$; temp range 154.6–313°C (tritoyl phosphate, Antoine eq., Weast 1972–73)
 $\log(P/\text{kPa}) = 11.81 - 5925/(T/K)$ (mixed isomers, Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 8.56 - 4535/(T/K)$ (*o*-TCP, Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 10.67 - 5787/(T/K)$ (*m*-TCP, Antoine eq., Riddick et al. 1986)
 $\log(P/\text{kPa}) = 13.24 - 5480/(T/K)$ (*p*-TCP, Antoine eq., Riddick et al. 1986)
 2.26×10^{-4} (*o*-TCP, Antoine eq., interpolated, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 8.565 - 4535/(T/K)$; temp range 293–700 K (*o*-TCP, Antoine eq., Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 11.8856 - 6104.5/[(T/K) - 10.81]$; temp range 398–530 K (*m*-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)
 $\log(P_L/\text{kPa}) = 10.245 - 5480/(T/K)$; temp range 388–530 K (*p*-TCP, Antoine eq. for liquid state, Stephenson & Malanowski 1987)
 3.07×10^{-4} , 1.25×10^{-4} (estimated from reported boiling points, Boethling & Cooper 1985)
 1.87×10^{-4} (quoted measured value, Boethling & Cooper 1985)
 6.10×10^{-6} (liquid P_L , GC-RT correlation, Hinckley et al. 1990)
 $\log(P/\text{mmHg}) = 21.1624 - 5.2756 \times 10^3/(T/K) - 3.3565 \cdot \log(T/K) + 8.666 \times 10^{-6} \cdot (T/K) - 2.9202 \times 10^{-9} \cdot (T/K)^2$; temp range 428–566 K (*o*-TCP, vapor pressure eq., Yaws et al. 1994)

Henry's Law Constant (Pa·m³/mol at 25°C):

- 0.0218 (calculated-P/C, Muir 1984, Muir et al. 1985)
 0.283, 0.172, 0.111 (calculated-P/C, Boethling & Cooper 1985)
 8.38 (*m*-TCP, gas stripping, Muir et al. 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

- 3.42 (HPLC-RT correlation, Veith 1979)
 5.11 (shake flask-concn ratio, Saeger et al. 1979)
 4.30, 4.65; 4.50 (RP-HPTLC- k' correlation, Renberg et al. 1980)
 5.107–5.12 (Muir 1984)
 5.10–5.30 (Bengtsson et al. 1986)

Bioconcentration Factor, $\log BCF$:

- 5.505, 4.45, 3.57, 3.57, 3.46 (*p*-TCP, ecological magnification factors for alga, snail, mosquito, fish and *Daphnia*, Metcalf 1976)
 2.88 (calculated for rainbow trout, Saeger et al. 1979)
 2.22 (fathead minnow, 32-d exposure, Veith et al. 1979)
 3.44, 3.15, 3.17 (*p*-TCP for rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)

- 2.89 (*p*-TCP for rainbow trout, calculated with hexane extract, Muir et al. 1983b)
 3.34, 2.97, 2.77 (*p*-TCP for fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
 2.85 (*p*-TCP, fathead minnow, calculated with hexane extractable radioactivity, Muir et al. 1983b)
 3.07, 2.89, 3.04 (*m*-TCP for rainbow trout: "initial rate" method, static test, Biofac, Muir et al. 1983b)
 2.49 (*m*-TCP for rainbow trout, calculated with hexane extractable radioactivity, Muir et al. 1983b)
 3.22, 2.77, 2.59 (*m*-TCP for fathead minnow: "initial rate" method, static test, Biofac, Muir et al. 1983b)
 2.66 (*m*-TCP, fathead minnow, calculated with hexane extract, Muir et al. 1983b)
 3.15, 2.89; 3.64 (rainbow trout: *p*-, *m*-TCP, static expt.; estimated- K_{OW} , Boethling & Cooper 1985)
 2.60 (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, log K_{OC} :

- 4.44 (calculated- K_{OW} , Muir 1984)
 3.86 (estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 496$ d (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis: $t_{1/2} = 73$ d and 52 d at 22°C for aryl phosphates (75% TCP and 18% TXP) in demineralized and river water (Wagemann et al. 1974; quoted, Boethling & Cooper 1985);

degradation $t_{1/2} = 3$ –4 d for *o*-, *m*-TCP and 5 d for *p*-TCP in Lake Ontario water (Howard & Dao 1979)
 second order alkaline hydrolysis rate constant $k = 0.025 \text{ M}^{-1} \text{ s}^{-1}$ (estimated, *p*-TCP, Wolfe 1980)

$t_{1/2} = 1.31$ h, 1.66 h for *m*-TCP and *p*-TCP, respectively, at pH 13.0 in acetone/water 1:1 solution (Muir et al. 1983b).

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

For *p*-TCP:

$k_1 = 25.8 \text{ h}^{-1}$, 21.8 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_1 = 15.9 \text{ h}^{-1}$, 7.80 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_2 = 0.0104 \text{ h}^{-1}$, 0.00963 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0106 \text{ h}^{-1}$, 0.0133 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

$k_2 = 0.0096 \text{ h}^{-1}$, 0.0077 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0070 \text{ h}^{-1}$, 0.0095 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

For *m*-TCP:

$k_1 = 28.8 \text{ h}^{-1}$, 24.0 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_1 = 18.2 \text{ h}^{-1}$, 12.2 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$, Muir et al. 1983b).

$k_2 = 0.0242 \text{ h}^{-1}$, 0.0229 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0115 \text{ h}^{-1}$, 0.0149 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

$k_2 = 0.0147 \text{ h}^{-1}$, 0.0117 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–144 h interval, Muir et al. 1983b).

$k_2 = 0.0085 \text{ h}^{-1}$, 0.0101 h^{-1} (fathead minnow, exposure concn 5, 50 $\mu\text{g/L}$ for 0–432 h interval, Muir et al. 1983b).

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

degradation $t_{1/2} = 3$ –4 d for *o*-, *m*-TCP and $t_{1/2} = 5$ d for *p*-TCP in Lake Ontario water (Howard & Dao 1979);

$t_{1/2} = 1.66$ h and 1.31 h in pH 13.0 acetone/water 1:1 solution (Muir et al. 1983b);

volatilization $t_{1/2}(\text{calc}) = 296$ d in 1 m deep water system (Muir 1984);

pseudo-first-order $t_{1/2} = 0.57$ d in pond water; moderate volatilization from water column with $t_{1/2} = 84$ d at 0.5-m depth (Muir et al. 1985).

Groundwater:

Sediment: $t_{1/2} = 39$ d in bottom sediment of a small pond (Muir et al. 1985).

Soil:

Biota: depuration $t_{1/2} = 135$ h in chironomid larvae (Muir et al. 1985);

elimination $t_{1/2} = 4$ d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

TABLE 15.1.4.1.7.1

Reported vapor pressures of tricresyl phosphate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)
$\log P = A - B/(C + T/K)$		(3)			
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)			
tri- <i>m</i> -cresyl phosphate				tri- <i>p</i> -cresyl phosphate	
Verhoek & Marshall 1939				Verhoek & Marshall 1939	
static and dynamic methods				static and dynamic methods	
$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa	$t/^{\circ}\text{C}$	P/Pa
Celluloid Corp. samples		Eastman Kodak samples			
80	0.00612	85.2	0.0132	92.0	0.0113
80	0.00604	95.4	0.0333	100.0	0.0267
80	0.00516	105.6	0.0749	110.0	0.0653
90	0.0177	115.8	0.1773	119.0	0.180
100.2	0.0461	126.0	0.448	119.0	0.189
109.9	0.1233			123.5	0.281
110.5	0.1276	eq. 1	P/ μmHg	124.0	0.283
114.0	0.212	A	13.982	125.0	0.249
114.0	0.208	B	5373	129.0	0.441
114.0	0.213			129.0	0.448
119.0	0.323	$\Delta H_v = 102.84$ kJ/mol		134.0	0.668
120.0	0.315			134.5	0.696
120.7	0.316			135.0	0.600
124.0	0.492			145.0	1.560
124.0	0.504				
125.9	0.509			eq. 1	P/ μmHg
128.8	0.739			A	15.223
129.0	0.785			B	5926
130.0	0.777				
131.0	0.809			$\Delta H_v = 113.43$ kJ/mol	
136.2	1.352				
eq. 1	P/ μmHg				
A	15.886				
B	6088				
$\Delta H_v = 116.54$ kJ/mol					

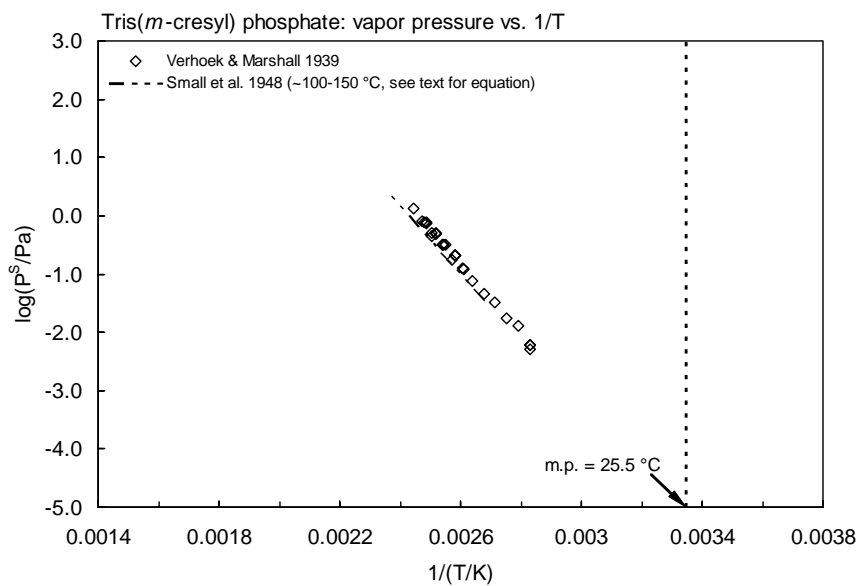


FIGURE 15.1.4.1.7.1a Logarithm of vapor pressure versus reciprocal temperature for *tris(m-cresyl)* phosphate.

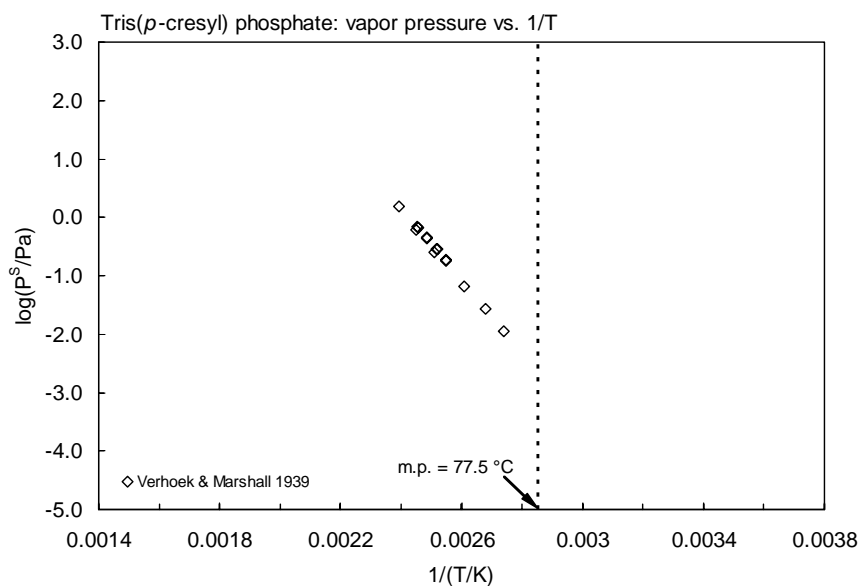
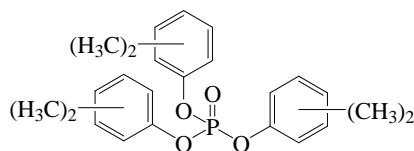


FIGURE 15.1.4.1.7.1b Logarithm of vapor pressure versus reciprocal temperature for *tris(p-cresyl)* phosphate.

15.1.4.1.8 Trixylenyl phosphate (TXP)



Common Name: Trixylenyl phosphate

Synonym: TXP

Chemical Name:

CAS Registry No: 25155-23-1

Molecular Formula: $C_{24}H_{27}O_4P$, $[(CH_3)_2C_6H_3]_3O_4P$

Molecular Weight: 410.442

Melting Point ($^{\circ}C$):

−20 (mixed isomers, Muir 1984)

Boiling Point ($^{\circ}C$):

261 (at 6 mmHg, Muir 1984)

225–295/6 mmHg, 248–265/4 mmHg, 270/3 mmHg (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56 J/mol K$), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.89 (shake flask-GC, Saeger et al. 1979)

0.89 (mixed isomers, Muir 1984)

Vapor Pressure (Pa at $25^{\circ}C$):

7.20×10^{-4} , 1.47×10^{-4} , 3.067×10^{-5} (estimated from reported boiling points, Boethling & Cooper 1985)

6.93×10^{-6} ($30^{\circ}C$, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.334, 0.0689, 0.0142, 0.00314 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

5.63 (shake flask-concn ratio, Saeger et al. 1979)

5.26 (RP-HPTLC- k' correlation, Renberg et al. 1980)

5.63 (Muir 1984)

5.70 (Boethling & Cooper 1985)

6.40–6.60 (Bengtsson et al. 1986)

Bioconcentration Factor, $\log BCF$:

3.15 (calculated for rainbow trout, Saeger et al. 1979)

4.04 (estimated from K_{OW} , Boethling & Cooper 1985)

3.11, 3.24, 3.28 (bleak, 28-d exposure, Bengtsson et al. 1986)

Sorption Partition Coefficient, $\log K_{OC}$:

4.44 (calculated- K_{OW} , Muir 1984)

3.67 (estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: 65% primary biodegradation in 14 weeks test duration for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} = 28\text{--}48$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Groundwater:

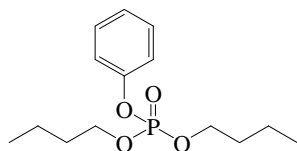
Sediment:

Soil:

Biota: eliminated $t_{1/2} = 4$ d or less (bleak, 28-d exposure, Bengtsson et al. 1986).

15.1.4.2 Triaryl/alkyl phosphates

15.1.4.2.1 Dibutyl phenyl phosphate (DBPP)



Common Name: Dibutyl phenyl phosphate

Synonym: DBPP

Chemical Name:

CAS Registry No: 2528-26-1

Molecular Formula: $C_{14}H_{23}O_4P$, $(C_4H_9)_2C_6H_5O_4P$

Molecular Weight: 286.303

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

200/20 mmHg (Muir 1984)

155/2 mmHg, 155/1 mmHg (quoted, Boethling & Cooper 1985)

Density (g/cm^3):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

96 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

66.7 (200 $^{\circ}C$, Muir 1984)

0.084, 0.0307 (estimated from boiling points, Boethling & Cooper 1985)

746* (170 $^{\circ}C$, GC-RT correlation, measured range 170–200 $^{\circ}C$, Skene & Krzymien 1995)

Henry's Law Constant (Pa $\cdot m^3/mol$ at $25^{\circ}C$):

0.253, 0.089 (estimated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{OW} :

4.27 (shake flask-concn ratio, Saeger et al. 1979)

3.23 (RP-HPTLC- k' correlation, Renberg et al. 1980)

Bioconcentration Factor, log BCF:

2.43 (calculated, Saeger et al. 1979)

3.04 (calculated- K_{OW} , Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC} :

3.70 (calculated- K_{OW} , Muir 1984)

2.56 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 0.4$ d (calculated, Muir 1984)

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 7$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

volatilization $t_{1/2} \sim 0.4$ d from 1 m deep water (Muir 1984).

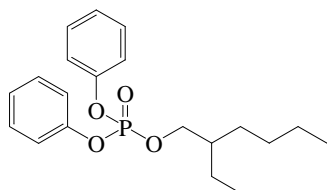
Groundwater:

Sediment:

Soil:

Biota:

15.1.4.2.2 2-Ethylhexyl diphenyl phosphate (EHDP)



Common Name: 2-Ethylhexyl diphenyl phosphate

Synonym: EHDP

Chemical Name:

CAS Registry No: 1241-94-7

Molecular Formula: $C_{20}H_{27}O_4P$, $C_8H_{17}(C_6H_5)_2O_4P$

Molecular Weight: 362.399

Melting Point ($^{\circ}C$):

−80 (Muir 1984)

Boiling Point ($^{\circ}C$):

181/0.6 mmHg (Wightman & Malaiyandi 1983)

239/1 mmHg (Muir 1984)

150/0.2 mmHg, 375/760 mmHg, 230/5 mmHg (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

1.9 (shake flask-GC, Saeger et al. 1979)

Vapor Pressure (Pa at $25^{\circ}C$):

4.0×10^{-3} , 3.47×10^{-3} , 1.87×10^{-3} (estimated from reported boiling points, Boethling & Cooper 1985)

Henry's Law Constant (Pa·m³/mol at $25^{\circ}C$):

1.60 (calculated-P/C, Muir 1982, 1984)

0.77, 0.648, 0.345 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, log K_{ow} :

5.73 (shake flask-concn ratio, Saeger et al. 1979)

5.00 (RP-HPLC- k' correlation, Renberg et al. 1980)

Octanol/Air Partition Coefficient, log K_{OA} :

Bioconcentration Factor, log BCF:

3.20 (calculated, Saeger et al. 1979)

3.17, 3.06; 3.12 (rainbow trout: calculated from rate constant ratio k_1/k_2 for exposure concn 5 and 50 $\mu g/L$; mean, Muir & Grift 1981)

3.52 (calculated- K_{ow} , Muir & Grift 1981)

4.11 (calculated- K_{ow} , Boethling & Cooper 1985)

Sorption Partition Coefficient, log K_{OC} :

4.49 (calculated- K_{ow} , Muir 1984)

3.49 (estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: half-life for 1 m deep water was estimated to be 7 d (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$k_1 = 48.5 \text{ h}^{-1}$, 33.0 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir & Grift 1981)

$k_2 = 0.0298 \text{ h}^{-1}$, 0.0294 h^{-1} (rainbow trout, exposure concn 5, 50 $\mu\text{g/L}$, Muir & Grift 1981)

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

rapid biodegradation $t_{1/2} = 2$ d in river water (quoted, Muir & Grift 1981);

volatilization $t_{1/2} \sim 7$ d for 1 m deep water (estimated, Muir 1984).

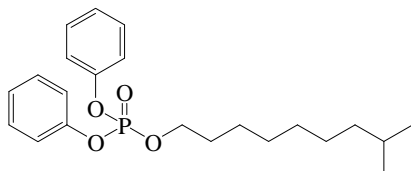
Groundwater:

Sediment:

Soil:

Biota:

15.1.4.2.3 Isodecyl diphenyl phosphate (IDDP)



Common Name: Isodecyl diphenyl phosphate

Synonym: IDDP

Chemical Name:

CAS Registry No: 29761-21-5

Molecular Formula: $C_{22}H_{31}O_4P$, $C_{10}H_{21}(C_6H_5)_2O_4P$

Molecular Weight: 390.452

Melting Point ($^{\circ}C$):

< -50 (Muir 1984)

Boiling Point ($^{\circ}C$):

245/10 mmHg (Boethling & Cooper 1985)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

0.75 (room temp, shake flask-GC, Saeger et al. 1979)

0.80 (Boethling & Cooper 1985)

Vapor Pressure (Pa at $25^{\circ}C$):

< 13.33, 66.7 (100, $150^{\circ}C$, Muir 1984)

2.133×10^{-3} (estimated from boiling point, Boethling & Cooper 1985)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

12.97 (calculated-P/C, Muir 1984)

1.013 (calculated-P/C, Boethling & Cooper 1985)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

5.44 (shake flask-concn ratio, Saeger et al. 1979)

3.31, 5.72; 5.42 (RP-HPTLC- k' correlation; mean, Renberg et al. 1980)

5.70 (quoted measured value, Boethling & Cooper 1985)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

3.04 (calculated, Saeger et al. 1979)

3.88 (estimated from solubility, Boethling & Cooper 1985)

Sorption Partition Coefficient, $\log K_{OC}$:

4.33 (calculated- K_{ow} , Muir 1984)

3.69 (soil, estimated from solubility, Boethling & Cooper 1985)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 1.3$ d for 1 m deep water system (Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in 10–21 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);
volatilization $t_{1/2} \sim 1.3$ d for 1 m deep water system (Muir 1984).

Groundwater:

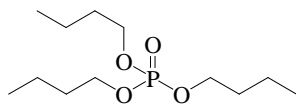
Sediment:

Soil:

Biota:

15.1.4.3 Trialkyl phosphate

15.1.4.3.1 Tributyl phosphate (TBP)



Common Name: Tributyl phosphate

Synonym: TBP, butyl phosphate

Chemical Name: tri-*n*-butyl phosphate

CAS Registry No: 126-73-8

Molecular Formula: $C_{12}H_{27}O_4P$; $(C_4H_9)_3O_4P$

Molecular Weight: 266.314

Melting Point ($^{\circ}C$):

< -80 (Dean 1985, Stephenson & Malanowski 1987)

Boiling Point ($^{\circ}C$):

289 (Lide 2003)

Density (g/cm^3):

0.972 ($25^{\circ}C$, Dean 1992)

0.976 (Riddick et al. 1986; Budavari 1989)

Molar Volume (cm^3/mol):

273.8 (Stephenson & Malanowski 1987)

Enthalpy of Vaporization, ΔH_v (kJ/mol):

14.67 (Dean 1992)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$ or as indicated. Additional data at other temperatures designated * are compiled at the end of this section):

422* (shake flask-electrometric titration, measured range 3.4 – $50^{\circ}C$, Higgins et al. 1959)

280 (shake flask-GC, Saeger et al. 1979)

390 (Riddick et al. 1986)

Vapor Pressure (Pa at $25^{\circ}C$ or as indicated and reported temperature dependence equations. Additional data at other temperatures designated * are compiled at the end of this section):

0.89 (extrapolated, Evans et al. 1930)

0.10, 2.0 (114, $160.2^{\circ}C$, Riddick et al. 1986)

$\log(P/kPa) = 7.7110 - 3206.5/(t/^{\circ}C + 273)$ (Antoine eq., Riddick et al. 1986)

$\log(P/kPa) = 7.7110 - 3206.5/(T/K)$ (Antoine eq., liquid phase, temp range 500 – 562 K, Stephenson & Malanowski 1987)

0.0202 (estimated from average air-borne concn, Skene & Krzymien 1995)

0.031, 0.015, 0.026, 0.030, 0.022 (extrapolated values from various reported Antoine equations, Skene & Krzymien 1995)

0.149* (gas saturation-GC, measured range 0 – $80^{\circ}C$; Skene & Krzymien 1995)

$\log(P/Pa) = 8.85629 - 1690.26/(T/K - 123.431)$; temp range 0 – $80^{\circ}C$, (Antoine eq. derived from exptl. data, gas saturation-GC, Skene & Krzymien 1995)

0.015 (TBP in Skydrol 500B-4 hydraulic fluid, gas saturation-GC, Skene & Krzymien 1995)

927–1060* ($170^{\circ}C$, GC-RT correlation, measured range 170 – $200^{\circ}C$. Skene & Krzymien 1995)

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

2513 (estimated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

- 4.004 (shake flask-concn ratio, Saeger et al. 1979)
- 3.99 (Sasaki et al. 1981)
- 4.004, 4.01 (quoted, Muir 1984)

Bioconcentration Factor, $\log BCF$:

- 2.28 (calculated, Saeger et al. 1979)
- 1.49–1.54 (killifish, 90-h exposure, static water system, Sasaki et al. 1981)
- 0.78–1.04 (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)
- 0.602–1.43 (killifish, static water system, Sasaki et al. 1982)
- 1.20–1.43 (killifish, 4–38 d exposure, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

- 3.56 (calculated- K_{OW} , Muir 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} = 0.4$ d for 1 m deep water system (calculated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water; $t_{1/2} < 28$ d for primary biodegradation rate from semicontinuous activated sludge studies (Saeger et al. 1979);

hydrolysis $t_{1/2} \sim 1$ yr for trialkyl phosphates (Wolfe 1980);

$t_{1/2} = 58$ h in the water containing killifish and more than 100 h for goldfish (Sasaki et al. 1981)

volatilization $t_{1/2} \sim 0.4$ d from 1 m deep water (estimated, Muir 1984).

Groundwater:

Sediment:

Soil:

Biota:

TABLE 15.1.4.3.1.1

Reported aqueous solubilities and vapor pressures of tributyl phosphate at various temperatures and the coefficients for the vapor pressure equations

$\log P = A - B/(T/K)$		(1)	$\ln P = A - B/(T/K)$		(1a)		
$\log P = A - B/(C + t/^{\circ}\text{C})$		(2)	$\ln P = A - B/(C + t/^{\circ}\text{C})$		(2a)		
$\log P = A - B/(C + T/K)$		(3)					
$\log P = A - B/(T/K) - C \cdot \log (T/K)$		(4)					
Aqueous solubility		Vapor pressure					
Higgins et al. 1959		Skene & Krzymien 1995					
shake flask-titration		GC-RT correlation					
t/°C	S/g·m ⁻³	t/°C	P/Pa	t/°C	P/Pa	t/°C	P/Pa
3.4	1075	0	0.004	different reference standards			
4.0	1012	5	0.01	170	1042	170	1060
5.0	957	15	0.04	185	1646	185	1849
13.0	640	25	0.15	200	4442	200	4102
25	422	35	0.39	Linear extrapolation eq.*		Linear extrapolation eq.*	
50	285	50	1.59	eq. 1	P/Pa	eq. 1	P/Pa
		65	7.17	A	12.336	A	12.333
		80	31.9	B	4124.2	B	4127.8
				170	927	170	993
		eq. 3	P/Pa	185	2179	185	1849
		A	8.85629	200	3030	200	3559
		B	1690.26	Linear extrapolation eq.*		Linear extrapolation eq.*	
		C	−123.431	eq. 1	P/Pa	eq. 1	P/Pa
				A	12.633	A	12.480
				B	4306.7	B	4215.3
				170	1109		
				185	2080		
				200	4408		
				Linear extrapolation eq.*			
				eq. 1	P/Pa		
				A	12.253		
				B	4080.7		
*regression eq. for extrapolation to temp range of gas saturation measurements 0–50°C							

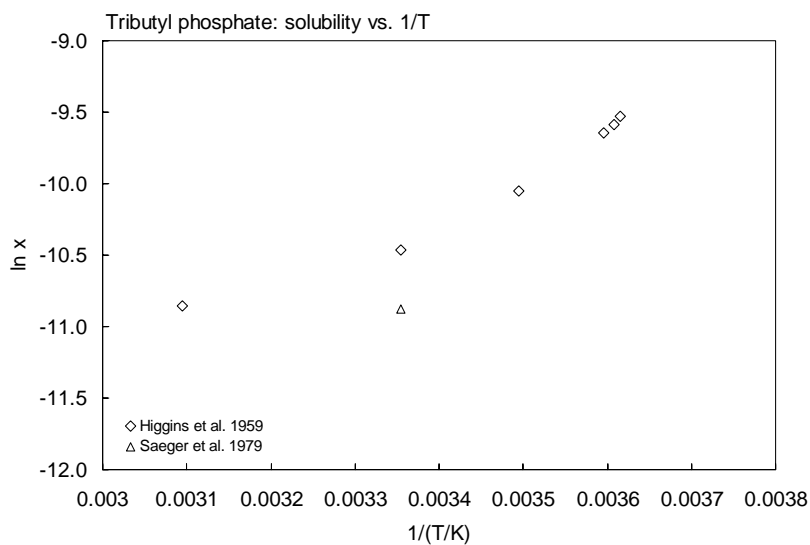


FIGURE 15.1.4.3.1.1 Logarithm of mole fraction solubility ($\ln x$) versus reciprocal temperature for tributyl phosphate.

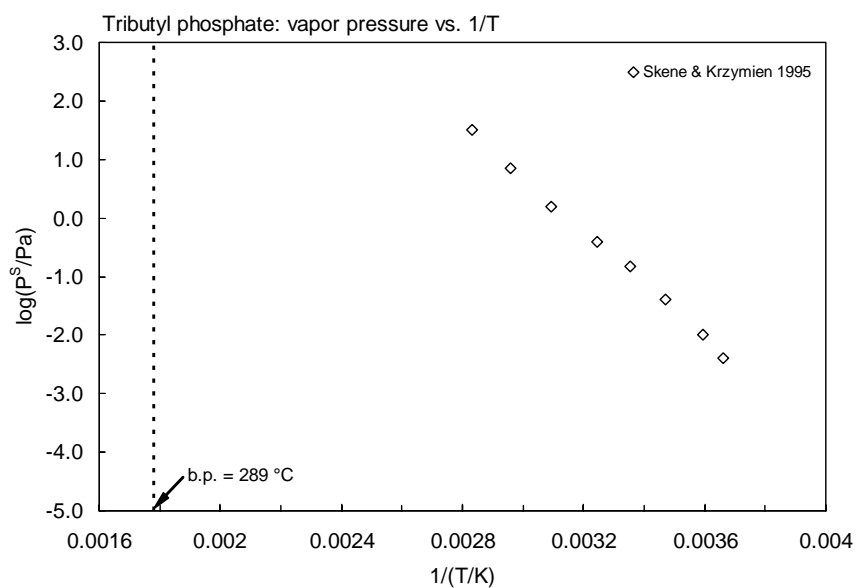
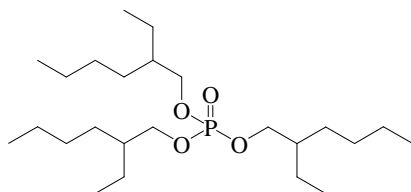


FIGURE 15.1.4.3.1.2 Logarithm of vapor pressure versus reciprocal temperature for tributyl phosphate.

15.1.4.3.2 *Tris(2-ethylhexyl) phosphate (TEHP)*

Common Name: Tris(2-ethylhexyl) phosphate

Synonym: TEHP

Chemical Name:

CAS Registry No: 78-42-2

Molecular Formula: $C_{24}H_{51}O_4P$, $(C_8H_{17})_3O_4P$

Molecular Weight: 434.633

Melting Point ($^{\circ}C$):

Boiling Point ($^{\circ}C$):

215 $^{\circ}C$ /4 mmHg (Aldrich Catalog 1989–99)

Density (g/cm³ at 20 $^{\circ}C$): 0.924 (Aldrich catalog 1998–99)

Molar Volume (cm³/mol):

Enthalpy of Vaporization, ΔH_v (kJ/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at 25 $^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F:

Water Solubility (g/m³ or mg/L at 25 $^{\circ}C$):

< 1000 (room temp, shake flask-GC, Saeger et al. 1979)

600 (practical grade, shake flask-nephelometry, Hollifield 1979)

Vapor Pressure (Pa at 25 $^{\circ}C$):

$\log(P/\text{mmHg}) = 12.85 - 5812/(T/K)$; exptl. data presented in graph and Antoine eq. (effusion, Small et al. 1948)
(See figure at the end of this section.)

1.10×10^{-5} (liquid P_L , GC-RT correlation, Hinckley et al. 1990)

Henry's Law Constant (Pa·m³/mol at 25 $^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{ow}$:

4.23 (shake flask-concn ratio, Saeger et al. 1979)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.40 (calculated, Saeger et al. 1979)

Sorption Partition Coefficient, $\log K_{oc}$:

3.68 (soil, calculated- K_{ow} , Muir 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

Half-Lives in the Environment:

Air:

Surface water: complete primary degradation in less than 7 d for river die-away studies when exposed to the natural microbial population of the water (Saeger et al. 1979).

Groundwater:

Sediment:

Soil:

Biota:

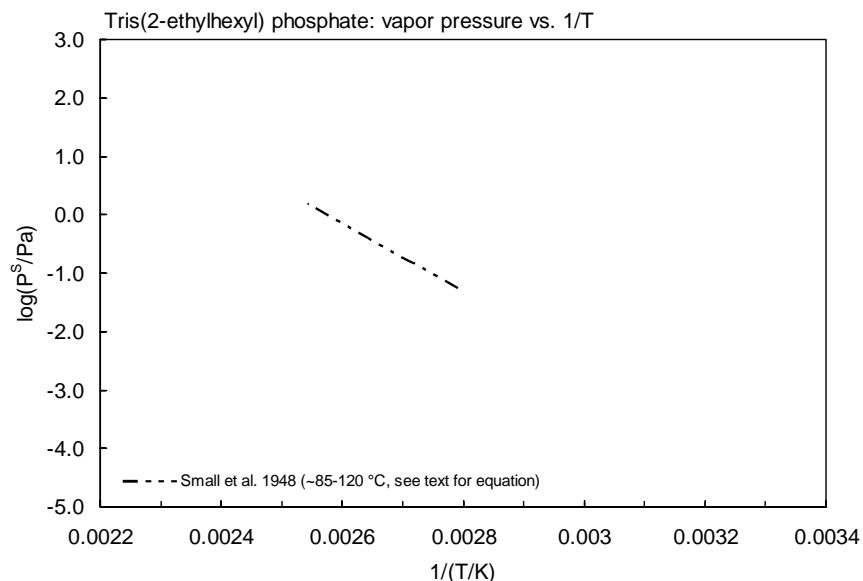
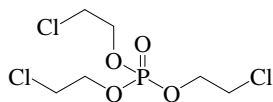


FIGURE 15.1.4.3.2.1 Logarithm of vapor pressure versus reciprocal temperature for *tris*(2-ethylhexyl) phosphate.

15.1.4.4 Trihaloalkyl phosphates

15.1.4.4.1 Tris(2-chloroethyl) phosphate (TCEP)



Common Name: Tris(2-chloroethyl) phosphate

Synonym: TCEP

Chemical Name:

CAS Registry No: 115-96-8

Molecular Formula: $C_6H_{12}Cl_3O_4P$, $(C_2H_4Cl)_3O_4P$

Molecular Weight: 285.490

Melting Point ($^{\circ}C$): -55

Boiling Point ($^{\circ}C$):

214/25 mmHg (Muir 1984)

330 (Stephenson & Malanowski 1987; Lide 2003)

Density (g/cm^3 at $20^{\circ}C$):

1.390 (Aldrich catalog 1989–99)

Molar Volume (cm^3/mol):

205.4 ($20^{\circ}C$, Stephenson & Malanowski 1987)

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} ($J/mol\ K$):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56\ J/mol\ K$), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

7000 (Eldefrawi et al. 1977; quoted, Sasaki et al. 1981)

7000 (quoted, Muir 1984)

Vapor Pressure (Pa at $25^{\circ}C$ and reported temperature dependence equations):

8.23 (interpolated-Antoine eq., Stephenson & Malanowski 1987)

$\log(P_L/kPa) = 4.346 - 1917/(T/K)$ (Antoine eq., temp range: 293–546 K, Stephenson & Malanowski 1987)

Henry's Law Constant ($Pa\cdot m^3/mol$ at $25^{\circ}C$):

0.00241 (calculated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, $\log K_{ow}$:

1.43 (shake flask, Sasaki et al. 1981)

1.48 (quoted, Muir 1984)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

2.40 (calculated, Saeger et al. 1979)

0.34 (killifish, 90-h exposure, static water system, Sasaki et al. 1981)

$-0.155, -0.046$ (goldfish, 90-h exposure, static water system, Sasaki et al. 1981)

0.36–1.10 (killifish, static water system, Sasaki et al. 1982)

0.041–1.10 (killifish, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

2.18 (calculated- K_{ow} , Muir 1984)

Environmental Fate Rate Constants, k , or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2} \sim 536$ d from 1 m deep water system (estimated, Muir 1984).

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

biological $t_{1/2} = 1.65$ h and elimination $t_{1/2} = 0.7$ h for killifish (Sasaki et al. 1982).

Half-Lives in the Environment:

Air:

Surface water: first order reduction process in river water, an estimated $t_{1/2} \sim 2.3$ d in Rhine River (Zoeteman et al. 1980);

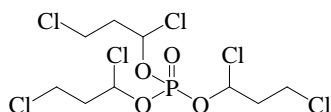
volatilization $t_{1/2}(\text{calc}) = 536$ d from 1 m deep water system (Muir 1984).

Groundwater:

Sediment:

Soil:

Biota: biological $t_{1/2} = 1.65$ h for accumulation, $t_{1/2} = 0.7$ h for elimination in killifish (Sasaki et al. 1982).

15.1.4.4.2 *Tris(1,3-dichloropropyl) phosphate (TDCPP)*

Common Name: Tris(1,3-dichloropropyl) phosphate

Synonym: TDCPP, TCPP, Fyrol FR-2, 1,3-dichloro-2-propanol phosphate (3:1), phosphoric acid tris(1,3-dichloro-2-propyl)ester, tris[2-chloro-1-(chloromethyl)ethyl]phosphate

Chemical Name:

Use: flame retardant

CAS Registry No: 40120-74-9

Molecular Formula: $C_9H_{15}Cl_6O_4P$, $(C_3H_5Cl_2)_3O_4P$

Molecular Weight: 430.906

Melting Point ($^{\circ}C$):

26.7 (Muir 1984)

viscous liquid (Budavari 1989)

Boiling Point ($^{\circ}C$):

236–237/5 mmHg (Muir 1984)

Density (g/cm^3 at $20^{\circ}C$):

1.5022 (Budavari 1989)

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 0.966

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

19.2 (Metcalf 1976)

7.0 (practical grade, shake flask-nephelometry, Hollifield 1979)

100 (Eldefrawi et al. 1977; quoted, Sasaki et al. 1981, Muir 1984)

~ 100 (Budavari 1989)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

Octanol/Water Partition Coefficient, $\log K_{OW}$:

3.76 (shake flask-concn ratio, Sasaki et al. 1981)

3.74 (quoted, Muir 1984)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

1.89–2.05 (killifish, 100-h exposure, static system, Sasaki et al. 1981)

0.48–0.70 (goldfish, 90-h exposure, static system, Sasaki et al. 1981)

1.67–2.03 (killifish, static system, Sasaki et al. 1982)

1.49–1.69 (killifish, 32-d exposure, continuous flow water system, Sasaki et al. 1982)

Sorption Partition Coefficient, $\log K_{OC}$:

3.41 (calculated- K_{OW} , Muir 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization:

Photolysis:

Oxidation:

Hydrolysis:

Biodegradation:

Biotransformation:

Bioconcentration, Uptake (k_1) and Elimination (k_2) Rate Constants:

$t_{1/2} = 31$ h in the water containing killifish and $t_{1/2} = 42$ h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

Half-Lives in the Environment:

Air:

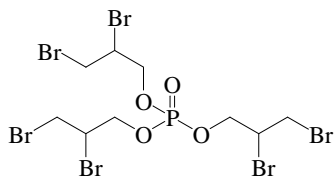
Surface water: $t_{1/2} = 31$ h in the water containing killifish and $t_{1/2} = 42$ h for goldfish, so that absorption occurred at similar rates in both fishes (Sasaki et al. 1981).

Groundwater:

Sediment:

Soil:

Biota: biological $t_{1/2} = 1.65$ h (killifish, Sasaki et al. 1982).

15.1.4.4.3 *Tris(2,3-dibromopropyl) phosphate (TDBPP)*

Common Name: Tris(2,3-dibromopropyl) phosphate

Synonym: TDBPP, Tris-BP, 2,3-dibromo-1-propanol phosphate(3:1), phosphoric acid tris(2,3-dibromopropyl) ester, Apex 462-3, Flammex AP, Firemaster: V-T 23P, Fyrol HB 32

Chemical Name:

Use: flame retardant

CAS Registry No: 126-72-7

Molecular Formula: $C_9H_{15}Br_6O_4P$, $(C_3H_5Br_2)_3O_4P$

Molecular Weight: 697.610

Melting Point ($^{\circ}C$):

5.5 (Muir 1984)

viscous liquid (Budavari 1989)

Boiling Point ($^{\circ}C$):

65/0.005 mmHg (Muir 1984)

Density (g/cm^3 at $20^{\circ}C$):

Molar Volume (cm^3/mol):

Enthalpy of Fusion, ΔH_{fus} (kJ/mol):

Entropy of Fusion, ΔS_{fus} (J/mol K):

Fugacity Ratio at $25^{\circ}C$ (assuming $\Delta S_{fus} = 56$ J/mol K), F: 1.0

Water Solubility (g/m^3 or mg/L at $25^{\circ}C$):

8.0 (practical grade, shake flask-nephelometry, Hollifield 1979)

1.60 (Muir 1984)

Vapor Pressure (Pa at $25^{\circ}C$):

Henry's Law Constant ($Pa \cdot m^3/mol$ at $25^{\circ}C$):

0.0108 (calculated-P/C, Muir 1984)

Octanol/Water Partition Coefficient, $\log K_{OW}$:

4.98 (HPLC-RT correlation, Veith et al. 1979)

4.39 (Muir 1984)

Octanol/Air Partition Coefficient, $\log K_{OA}$:

Bioconcentration Factor, $\log BCF$:

0.44 (calculated- K_{OW} , Veith et al. 1979)

Sorption Partition Coefficient, $\log K_{OC}$:

3.76 (calculated- K_{OW} , Muir 1984)

Environmental Fate Rate Constants, k, or Half-Lives, $t_{1/2}$:

Volatilization: $t_{1/2}$ (calc) = 1.9 d in 1 m deep water system (Muir 1984).

Half-Lives in the Environment:

Surface water: volatilization $t_{1/2}$ (calc) = 1.9 d in 1 m deep water system (Muir 1984).

15.2 SUMMARY TABLES AND QSPR PLOTS

TABLE 15.2.1

Summary of physical properties of esters and phthalate esters

Compound	CAS no.	Molecular formula	Molecular weight, MW g/mol	m.p. °C	b.p. °C	Fugacity ratio, F at 25°C*	Molar volume, V _M	
							cm ³ /mol	
							MW/ρ at 20°C	Le Bas
Aliphatic esters:								
Methyl formate	107-31-3	HCO ₂ CH ₃	60.052	−99	31.7	1	61.64	62.6
Ethyl formate	109-94-4	HCO ₂ C ₂ H ₅	74.079	−79.6	54.4	1	80.35	86.4
Propyl formate	110-74-7	C ₄ H ₈ O ₂	88.106	−92.9	80.9	1	97.30	110.8
Butyl formate	592-84-7	C ₅ H ₁₀ O ₂	102.132	−91.9	106.1	1		133
Isobutyl formate	542-55-2	C ₅ H ₁₀ O ₂	102.132	−95.8	98.2	1		133
Methyl acetate	79-20-9	(CH ₃) ₂ CO ₂	74.079	−98.25	56.87	1	79.30	84.8
Vinyl acetate	108-05-4	C ₄ H ₆ O ₂	86.09	−93.2	72.8	1	92.40	101.2
Allyl acetate	591-87-7	C ₅ H ₈ O ₂	100.117		103.5	1		125.6
Ethyl acetate	141-78-6	C ₄ H ₈ O ₂	88.106	−83.8	77.11	1	97.83	108.6
Propyl acetate	109-60-4	C ₅ H ₁₀ O ₂	102.132	−93	101.54	1	115.04	133
Butyl acetate	123-86-4	C ₆ H ₁₂ O ₂	116.158	−78	126.1	1	132.54	155.2
Isobutyl acetate	110-19-0	C ₆ H ₁₂ O ₂	116.158	−98.8	116.5	1		155.2
Pentyl acetate	628-63-7	C ₇ H ₁₄ O ₂	130.185	−70.8	149.2	1	148.51	177.4
Isopentyl acetate	123-92-2	C ₇ H ₁₄ O ₂	130.185	−78.5	142.5	1		177.4
Hexyl acetate	142-92-7	C ₈ H ₁₆ O ₂	144.212	−80.9	171.5	1		199.6
Cyclohexyl acetate	622-45-7	C ₈ H ₁₄ O ₂	142.196		173			177.2
2-Ethylhexyl acetate	103-09-3	C ₁₀ H ₂₀ O ₂	172.265	−80	199	1		244
Benzyl acetate	140-11-4	C ₉ H ₁₀ O ₂	150.174	−51.3	213	1		177.2
Ethyl propionate	105-37-3	C ₅ H ₁₀ O ₂	102.132	−73.9	99.1	1		130.8
Ethyl butyrate	105-54-4	C ₆ H ₁₂ O ₂	116.158	−98	121.3	1		153
Methyl acrylate	96-33-3	C ₄ H ₆ O ₂	86.09	< −75	80.7	1	90.29	99.6
Ethyl acrylate	140-88-5	C ₅ H ₈ O ₂	100.117	−71.2	99.4	1	108.42	123.8
Methyl methacrylate	80-62-6	C ₅ H ₈ O ₂	100.117	−47.55	100.5	1	106.06	121.8
Ethyl methacrylate	97-63-2	C ₆ H ₁₀ O ₂	114.142		117			145.6
Aromatic esters:								
Methyl benzoate	93-58-3	C ₈ H ₈ O ₂	136.149	−12.4	199	1	125.07	151.2
Ethyl benzoate	93-89-0	C ₉ H ₁₀ O ₂	150.174	−34	212	1	142.87	175
Propyl benzoate	2315-68-6	C ₁₀ H ₁₂ O ₂	164.201	−51.6	211	1	160.48	199.4
Phenyl benzoate	93-99-2	C ₁₃ H ₁₀ O ₂	198.217	71	314	0.354		221.4
Benzyl benzoate	120-51-4	C ₁₄ H ₁₂ O ₂	212.244	21	323.5	1		243.6

Phthalate esters:

Dimethyl phthalate (DMP)	131-11-3	C ₁₀ H ₁₀ O ₄	194.184	5.5	283.7	1	163.11	206.4
Diethyl phthalate (DEP)	84-66-2	C ₁₂ H ₁₄ O ₄	222.237	-40.5	295	1	198.87	254
Diallyl phthalate (DAP)	131-17-9	C ₁₄ H ₁₄ O ₄	246.259	-77	290		219.68	288
Di- <i>n</i> -propyl phthalate (DnPP)	131-16-8	C ₁₄ H ₁₈ O ₄	250.291	-31.0	304.5	1		302.8
Di-isopropyl phthalate (DIPP)	605-45-8	C ₁₄ H ₁₈ O ₄	250.291	liquid		1		302.8
Di- <i>n</i> -butyl phthalate (DBP)	84-74-2	C ₁₆ H ₂₂ O ₄	278.344	-35	340	1	265.85	347.2
Di-isobutyl phthalate (DIBP)	84-69-5	C ₁₆ H ₂₂ O ₄	278.344		296.5	1		347.2
Dipentyl phthalate (DPP)	131-18-0	C ₁₈ H ₂₆ O ₄	306.397	< -54.5	342	1		391.6
Dihexyl phthalate (ΔHP)	84-75-3	C ₂₀ H ₃₀ O ₄	334.45	-27.4		1	337.83	436
Butyl 2-ethylhexyl phthalate (BOP)	85-69-8	C ₂₀ H ₃₀ O ₄	334.45	-37		1		436
Di- <i>n</i> -octyl phthalate (DOP)	117-84-0	C ₂₄ H ₃₈ O ₄	390.557	25		1	399.34	524.8
Di-isooctyl phthalate (DIOP)	27554-26-3	C ₂₄ H ₃₈ O ₄	390.557		370	1		524.8
<i>bis</i> (2-Ethylhexyl) phthalate (DEHP)	117-81-7	C ₂₄ H ₃₈ O ₄	390.557	-55	384	1	396.79	524.8
Di (hexyl, octyl, decyl) phthalate	39289-94-6	C ₂₅ H ₄₀ O ₄	404.583	-4		1		547.0
Di-isononyl phthalate (DINP)	9727830	C ₂₆ H ₄₂ O ₄	418.609	-48		1	420.71	569.2
Di-isodecyl phthalate (DIDP)	26761-40-0	C ₂₈ H ₄₆ O ₄	446.663	-50		1		613.6
Diundecyl phthalate (DUP)	3648-20-2	C ₃₀ H ₅₀ O ₄	474.716	35.5		0.789		658.0
Ditridecyl phthalate (DTDP)	43617	C ₃₄ H ₅₈ O ₄	530.823	-37		1		746.8
Butyl benzyl phthalate (BBP)	85-68-7	C ₁₉ H ₂₀ O ₄	312.360	-35	370	1		369.2

Phosphate esters:

<i>t</i> -Butylphenyl diphenyl phosphate	56803-37-3	C ₂₂ H ₂₃ O ₄ P	382.389	-21		1		
Cresyl diphenyl phosphate (CDP)	26444-49-5	C ₁₉ H ₁₇ O ₄ P	340.309					
Isopropylphenyl diphenyl phosphate (IPDP)	28108-99-8	C ₂₁ H ₂₁ O ₄ P	368.362	-26		1		
4-Cumylphenyl diphenyl phosphate	84602-56-2	C ₂₇ H ₂₅ O ₄ P	444.458					
Nonylphenyl diphenyl phosphate	13418387	C ₂₇ H ₃₃ O ₄ P	452.522					
Triphenyl phosphate (TPP)	115-86-6	C ₁₈ H ₁₅ O ₄ P	326.283	50.5		0.562		
Tricresyl phosphate (TCP)	1330-78-5	C ₂₁ H ₂₁ O ₄ P	368.362					
Trixylenyl phosphate (TXP)	25155-23-1	C ₂₄ H ₂₇ O ₄ P	410.442					
Dibutyl phenyl phosphate (DBPP)	2528-26-1	C ₁₄ H ₂₃ O ₄ P	286.303					
2-Ethylhexyl diphenyl phosphate	1241-94-7	C ₂₀ H ₂₇ O ₄ P	362.399	-80		1		
Isodecyl diphenyl phosphate (IDDP)	29761-21-5	C ₂₂ H ₃₁ O ₄ P	390.452	< -50		1		
Tributylphosphate (TBP)	126-73-8	C ₁₂ H ₂₇ O ₄ P	266.314	< -80		1		
Tris(2-ethylhexyl) phosphate	78-42-2	C ₂₄ H ₅₁ O ₄ P	434.633					
Tris(2-chloroethyl) phosphate	115-96-8	C ₆ H ₁₂ Cl ₃ O ₄ P	285.49			1		
Tris(1,3-dichloropropyl) phosphate	40120-74-9	C ₉ H ₁₅ Cl ₆ O ₄ P	430.906	26.7		0.962		
Tris(2,3-dibromopropyl) phosphate	126-72-7	C ₉ H ₁₅ Br ₆ O ₄ P	697.61	5.5		1		

* Assuming ΔS_{fus} = 56 J/mol K.

TABLE 15.2.2
Summary of selected physical-chemical properties of esters and phthalate esters at 25°C

Compound	Selected properties						Henry's law constant		
	Vapor pressure		Solubility			log K _{OW}	H/(Pa·m ³ /mol)		
	P ^S /Pa	P _L /Pa	S/(g/m ³)	C ^S /(mol/m ³)	C _L /(mol/m ³)		calcd P/C	exptl (a)	exptl (b)
Aliphatic esters:									
Methyl formate	78060	78060	230000	3830	3830	−0.26	20.38		
Ethyl formate	32370	32600	118000	1593	1593	0.23	20.32		
Propyl formate	11030	11030	20500	232.7	232.7	0.73	47.40		
Butyl formate	3840	3840							
Isobutyl formate	5343	5400	10000	97.91	97.91		54.57		
Methyl acetate	28800	28800	245000	3307	3307	0.23	8.708	0.65	13.06
Vinyl acetate	14100	14100	20000	232.3	232.3	0.73	60.69		
Allyl acetate	6130	6130							
Ethyl acetate	12600	12600	80800	917.1	917.1		13.74		17.2
Propyl acetate	4500	4500	21000	205.6	205.6	1.24	21.88		22.09
Butyl acetate	1600	1600	6000	51.65	51.65	1.82	30.98		29.506
Isobutyl acetate	2860	2860	6300	54.24	54.24	1.6	52.73		
Pentyl acetate	550	550	1700	13.06	13.06	2.42	42.12		35.94
Isopentyl acetate	600	600	2000	15.36	15.36	2.13	39.06		
Hexyl acetate	670	670	500	3.446	3.467		193.2		
2-Ethylhexyl acetate	53	53	98.4	0.5712	0.5712	3.72	92.79		
Phenyl acetate						1.49			
Benzyl acetate	189	189	sl. sol.	sl. sol.		1.96			
Methyl propionate	11600	11600	62370	707.9	707.9		16.39	17.6	
Ethyl propionate	4966	4966	19200	188.0	188.0	1.21	26.42		
Methyl butyrate								20.82	
Ethyl butyrate	2300	2300	6500	55.96	55.96	1.73	41.10		
Methyl pentanoate								32.22	
Methyl hexanoate								37.18	
Methyl octanoate								79.32	
Methyl acrylate	11000	11000	49400	573.8	573.8	0.8	19.17		
Ethyl acrylate	5100	5100	15000	149.82	149.82	1.33	34.041		
Methyl methacrylate	5100	5100	15600	155.8	155.8	1.38	32.73		
Ethyl methacrylate						1.94			

Aromatic esters:

Methyl benzoate	52.58	52.28	2100	15.42	15.42	2.2	3.389
Ethyl benzoate	24	24	350	2.331	2.331	2.64	10.30
Propyl benzoate	100	100				3.18	
Phenyl benzoate		0.416				3.59	
Benzyl benzoate	0.043	0.043	16	0.0754	0.0754	3.97	0.5704

Phthalate esters:

Dimethyl phthalate (DMP)	0.22	0.22	4000	20.60	20.60	2.12	0.0107
Diethyl phthalate (DEP)	0.22	0.22	1080	4.859	4.859	2.47	0.0453
Di- <i>n</i> -butyl phthalate (DBP)	0.00187	0.00187	11.2	0.0402	0.0402	4.72	0.0465
Di- <i>n</i> -octyl phthalate (DOP)	1.33×10^{-5}	1.33×10^{-5}	0.0005	1.28×10^{-6}	1.28×10^{-6}	8.06	10.39
<i>bis</i> (2-Ethylhexyl)-phthalate	1.33×10^{-5}	1.33×10^{-5}	0.003	7.68×10^{-6}	7.68×10^{-6}	7.5	1.731
Butyl benzyl phthalate	0.00115	0.00115	2.69	0.0086	0.0086	4.60	0.1335

(a) Buttery et al. 1969

(b) Kieckbusch & King 1979

TABLE 15.2.3

Suggested half-life classes for esters and phthalate esters in various environmental compartments at 25°C

Compound	Air class	Water class	Soil class	Sediment class
Aliphatic esters:				
Methyl formate	3	3	4	5
Ethyl formate	3	3	4	5
Butyl formate	3	3	4	5
Methyl acetate	3	3	4	5
Vinyl acetate	3	3	4	5
Allyl acetate	3	3	4	5
Ethyl acetate	3	3	4	5
Propyl acetate	3	3	4	5
Butyl acetate	3	3	4	5
Pentyl acetate	3	3	4	5
Methyl methacrylate	2	3	4	5
Phthalate esters:				
Dimethyl phthalate (DMP)	4	5	6	7
Diethyl phthalate (DEP)	4	5	6	7
Di- <i>n</i> -butyl phthalate (DBP)	3	5	6	7
<i>bis</i> (2-Ethylhexyl)-phthalate (DEHP)	3	5	6	7
Butyl benzyl phthalate (BBP)	3	5	6	7

where,

Class	Mean half-life (hours)	Range (hours)
1	5	< 10
2	17 (~ 1 day)	10–30
3	55 (~ 2 days)	30–100
4	170 (~ 1 week)	100–300
5	550 (~ 3 weeks)	300–1,000
6	1700 (~ 2 months)	1,000–3,000
7	5500 (~ 8 months)	3,000–10,000
8	17000 (~ 2 years)	10,000–30,000
9	~ 5 years	> 30,000

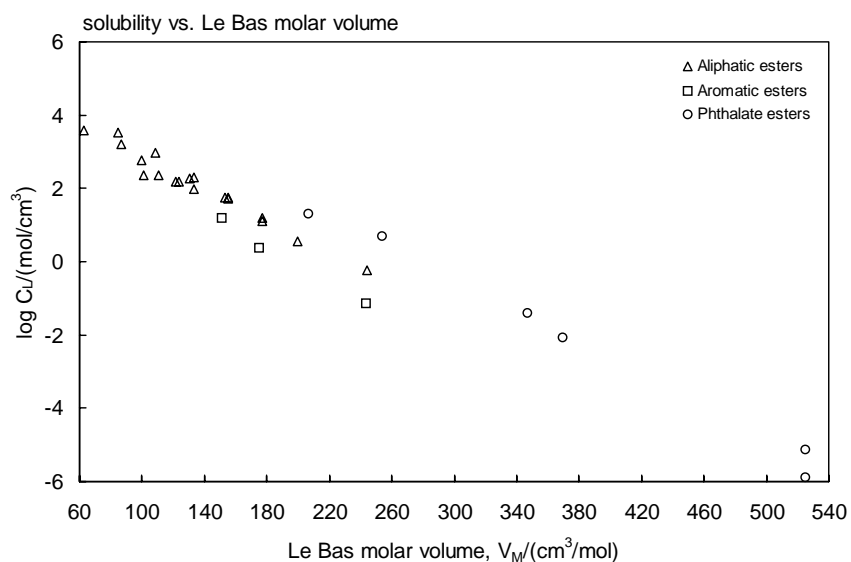


FIGURE 15.2.1 Molar solubility (liquid or supercooled liquid) versus Le Bas molar volume for esters.

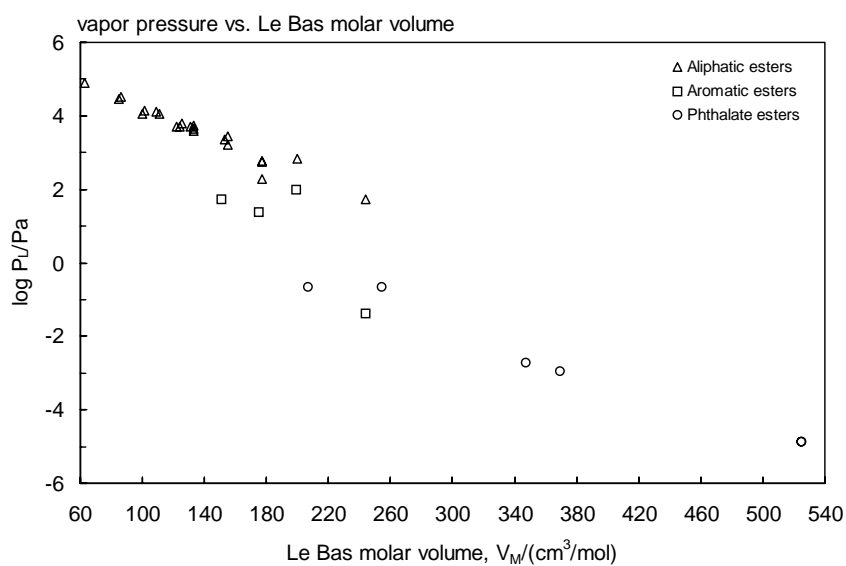


FIGURE 15.2.2 Vapor pressure (liquid or supercooled liquid) versus Le Bas molar volume for esters.

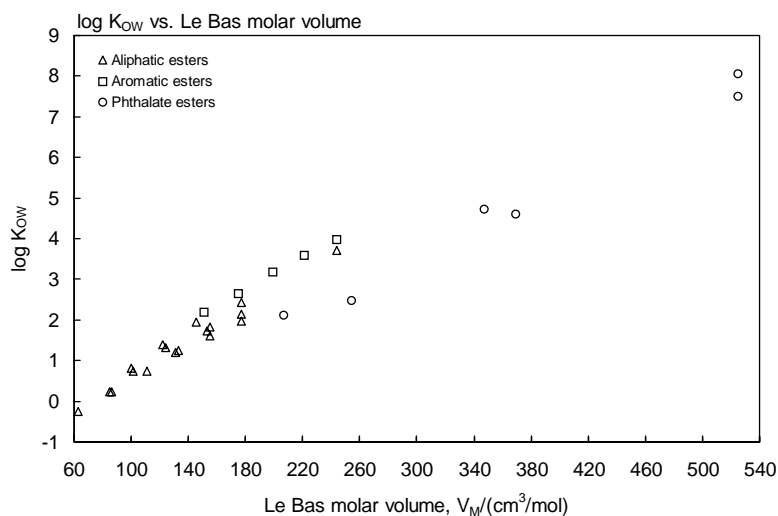


FIGURE 15.2.3 Octanol-water partition coefficient versus Le Bas molar volume for esters.

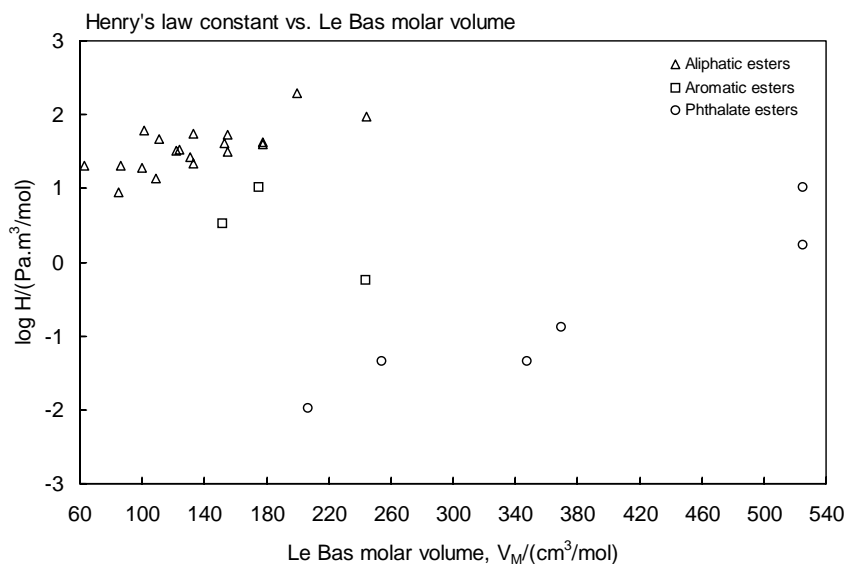


FIGURE 15.2.4 Henry's law constant versus Le Bas molar volume for esters.

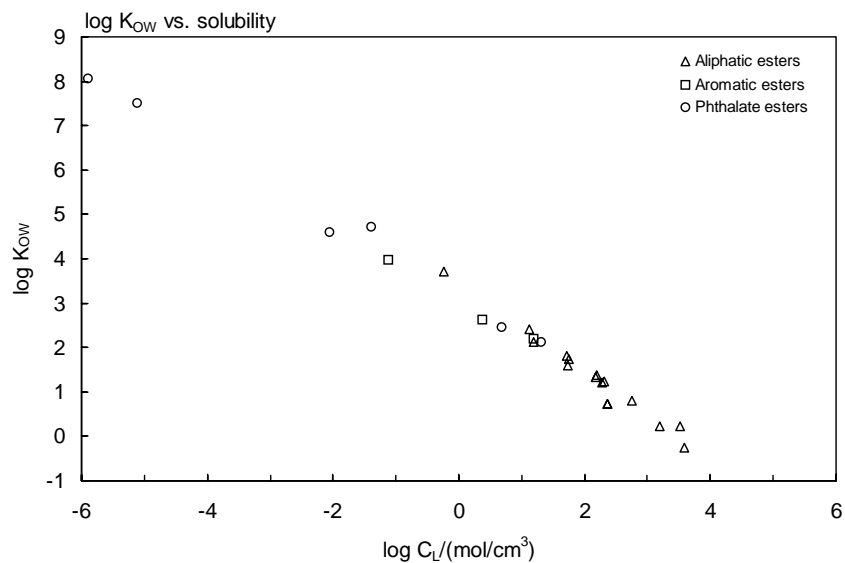


FIGURE 15.2.5 Octanol-water partition coefficient versus molar solubility (liquid or supercooled liquid) for esters.

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